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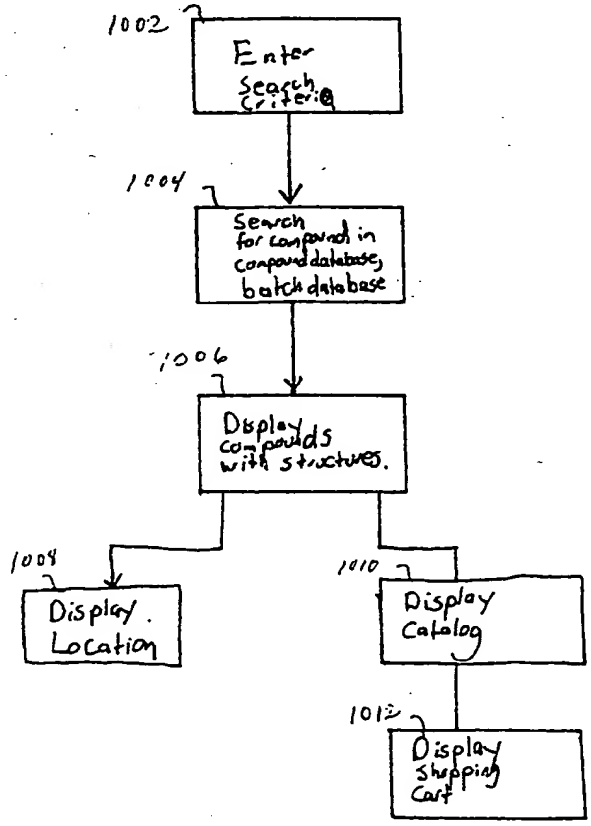
(54) Title: CHEMICAL COMPOUND INFORMATION SYSTEM

(57) **Abstract**

Systems and methods for managing chemical compound information. Chemical compound tracking and purchasing systems may be provided. A user interface (1002) allows for queries to identify compounds (1004) available internally to the organization and for orders from external sources for compounds that are unavailable internally. Background processing of compound characteristics as stored in a chemical compound database (1004) may be provided (1006).



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CHEMICAL COMPOUND INFORMATION SYSTEM

BACKGROUND OF THE INVENTION

The present invention relates to information systems and more particularly to information systems for chemical compounds.

Operation of the modern chemical laboratory environment requires the management of large numbers of chemical compound containers. These containers may be dispersed over thousands of locations. A researcher or chemist desiring a given chemical compound may be aware of chemical compounds found at his or her location or possibly at nearby locations but is likely to be unaware of chemical compounds available within his or her organization. He or she may conduct a search by physically scanning available contents at many locations or by making successive telephone calls to personnel throughout the organization. It may be more time efficient and thus cheaper to simply order the chemical compound from an external source even if the chemical compound is already available internally.

Even ordering from an external source is complicated by the need to search through numerous supplier catalogs which may not be up to date. After locating the catalog information, completing an order generally requires contacting the supplier by telephone during the supplier's business hours.

A related management problem concerns collecting and maintaining information on the characteristics of chemical compounds. For the purpose of identifying chemical compounds for particular purposes including pharamaceutical purposes, it would be desirable to maintain a chemical compound database that stores for each of many chemical compounds information including: 1) the three dimensional structure of the compound, 2) identification of pharmacaphores of the compound, and 3) a specification of the compound structure that does not include disconnected salt fragments.

SUMMARY OF THE INVENTION

By virtue of the present invention, systems and methods for managing chemical compound information are provided. One embodiment provides a chemical compound tracking and purchasing system. A container database is maintained identifying chemical compound containers available within an organization. A integrated user interface

allows for queries to identify compounds available internally to the organization and for orders from external sources for compounds that are unavailable internally.

Another embodiment of the invention provides background processing of compound characteristics as stored in a chemical compound database. When a chemical compound is registered to a database, its two-dimensional chemical structure is also registered. One or more autonomous processes take this two-dimensional chemical structure as an input to generate additional compound characteristic information to add to the compound database. For example, a first autonomous process may remove salts from stored two-dimensional structures. The removal of salts facilitates searching for useful compounds because salt substructures do not normally affect the ability of one compound to bond with another. A second autonomous process may remove protective groups from the stored structures. These are groups that cleave during synthesis and it is useful to remove them from the compound database to facilitate the evaluation of database products. A third autonomous process may determine a possible three-dimensional structure for each compound, an example of information useful in identifying compounds having desired pharmaceutical characteristics. A fourth autonomous process may identify pharmacaphoric groupings in the stored two-dimensional structures. Knowledge of the pharmacaphores found within each compound greatly facilitates searching for compounds having desired pharmaceutical characteristics.

Another embodiment of the present invention provides for chemical compound registration system having a web-based interface. The web-based interface facilitates entering information about chemical compounds from any location on a network.

A further understanding of the nature and advantages of the inventions herein may be realized by reference to the remaining portions of the specification and the attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 depicts a computer system suitable for implementing one embodiment of the present invention.

Fig. 2 depicts a computer network suitable for implementing one embodiment of the present invention.

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to one embodiment of the present invention.

Fig. 4 is a flowchart describing steps of an overall background process for enriching a chemical compound database in the background according to one embodiment of the present invention.

Fig. 5 is a flowchart describing steps of removing salts from a chemical compound according to one embodiment of the present invention.

Fig. 6 depicts a compound with pharmacaphoric groupings marked and with a salt removed.

Fig. 7 depicts a simplified representation of a laboratory facility.

Fig. 8 depicts a scanner as would be used in one embodiment of the present invention.

Fig. 9 depicts a flowchart describing steps of tracking chemical compound containers according to one embodiment of the present invention.

Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention.

Figs. 11A-11F depict a user interface for locating and purchasing chemical compounds according to one embodiment of the present invention.

Fig. 12 depicts a configuration of pharmacaphoric groupings.

DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides a chemical compound information system. In certain embodiments, the information system includes a chemical compound tracking and purchase system. In certain other embodiments, the chemical compound information system includes a chemical compound registry for registering information about new compounds. This registry may have a web-based interface. Once compounds are registered to a database, background processing may enrich the database with useful information about the compounds such as, e.g., three-dimensional structure, pharmacaphoric groupings, and information about included salts.

Representative Hardware

Fig. 1 shows basic subsystems of a computer system suitable for use with the present invention. In Fig. 1, computer system 10 includes bus 12 which interconnects major subsystems such as central processor 14, system memory 16, input/output (I/O) controller 18, an external device such as a printer 20 via parallel port 22, display screen 24 via display adapter 26, serial port 28, keyboard 30, fixed disk drive 32 and floppy disk drive 33 operative to receive a floppy disk 33A. Many other devices can be connected such as scanning device 34 connected via I/O controller 18, a network interface 35, a mouse 38 connected via serial port 28. Many other devices or subsystems (not shown) may be connected in a similar manner. Also, it is not necessary for all of the devices shown in Fig. 1 to be present to practice the present invention, as discussed below. The devices and subsystems may be interconnected in different ways from that shown in Fig. 1. The operation of a computer system such as that shown in Fig. 1 is readily known in the art and is not discussed in detail in the present application. Source code to implement the present invention may be operably disposed in system memory 16 or stored on storage media such as fixed disk 32 or floppy disk 33A.

Fig. 2 depicts a computer network 200 suitable for implementing the present invention. A central station 202 maintains databases as described herein. Central station 202 is preferably a Unix or Windows NT server such as an ORGIN 2000 server available from Silicon Graphics, Inc. of Mountain View, California. Central station 202 operates databases as described below and preferably provides external access to these databases using standard well-known Internet protocols such as HTTP. Database operation may also be divided among multiple central stations.

A plurality of remote stations 204 may access the databases of central station 202 using HTTP. Database access may be for searching for needed compounds or for registering new compounds. Remote stations 204 operate standard web browsing software such as Netscape Navigator or Microsoft Internet Explorer. Remote stations 204 may be implemented on a wide variety of computer platforms that support such browsing software. Any time of network may interconnect central station 202 including LANs, WANs, the Internet, an intranet, or any combination of these.

Databases Operated

A chemical compound information system according to the present invention may maintain various databases. A chemical compound database may include records corresponding to individual chemical compounds. Each record includes one or more of the representative fields shown in Table 1.

TABLE 1

FIELD	INFORMATION
MOLREGNO	Unique registration number for molecule
MOLNAME	Molecule name
CONV_NAME	Conventional name
IUPAC_NAME	IUPAC name
MOLFORMULA	Molecular formula
MIN_MWT	Minimum molecular weight
MAX_MWT	Maximum molecular weight
REGNO	Organization-wide reg. no.
PUBLISH	Make available to other parts of organization--yes or no?
STORAGE_COND	Storage conditions
SOLUBILITY	Solubility
HANDLEPRECAUT	Handling precautions
STEREO_ISOMER	Whether or not there are stereo isomers
GEOM_ISOMER	Whether or not there are geometric isomers
SAM_COMMENT	Comment
LEGACY_DATE	
PARENT_REGNUM	Registration number of synthesis predecessor

TABLE 1	
FIELD	**INFORMATION**
NUMSPECIFIC_STRUCT	Status of background calculations

Each molecule has a unique registration number, "REGNO." The remaining fields are self-explanatory. "NUMSPECIFIC_STRUCT" indicates the status of background calculations that will be described below. The information in the remaining fields is self-explanatory in the table. The present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

Another database indexed by MOLREGNO may include the two-dimensional structure for each molecule. There are many possibilities for denoting the two-dimensional structure. In one embodiment, a list of atoms and bonds is given to identify the two-dimensional structure.

A batch database may list the chemical compound containers that are available, e.g. within an organization without resort to an external ordering process. Each container within the organization may have a record within the batch database. Table 2 shows representative fields of a record within the batch database. "LOTNUM" and "REGNO" serve as a key to the batch database. It is contemplated that each container be marked with a bar code that has an associated bar code number. Certain fields concern the source of the batch. Other fields identify personnel responsible for the batch. There are also fields to represent whether certain analysis procedures have been conducted and to represent the results. Again, the present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

TABLE 2	
FIELD	**INFORMATION**
REGNO	Reg. number for molecule
LOTNUM	Unique reg. number for batch

TABLE 2

FIELD	INFORMATION
CHEMIST	Responsible chemist
SUPERVISOR	Responsible supervision
CHEM_SOURCE	Identify source
CATALOG NOTEBOOK	Catalog ID or NOTEBOOK#
VENDOR_NAME	Name of vendor
BARCODE	Barcode number
AMOUNT	Amount
AMOUNT_UNIT	Amount units
PURITY_PERCENT	Purity percentage
QC_METHOD	Quality control analysis method used
QC_HPLC	Chromatography applied?
HPLC_FILENAME	Chromatography results file
QC_MS	Mass spectrometry applied?
MS_FILENAME	Mass spectrometry results file
QC_C13NMR	C_{13} NMR applied?
C13NMR_FILENAME	C_{13} NMR results file
QC_HNMR	H NMR applied?
HNMR_FILENAME	H NMR results file
MPLOW	Low melting point
MPHIGH	High melting point
MP_COMMENT	Comment on melting point
BPLOW	Low boiling point
BPHIGH	High boiling point
BP_COMMENT	Boiling point comment
OPTROT	Optical rotation information

TABLE 2	
FIELD	**INFORMATION**
PHYS_STATE	Liquid, solid, or gas
BATCH_COMMENT	Batch comment
HANDLE_PRECAUT	Handling precautions
STOR_COND	Storage conditions
ASSIGNED_OTHER_ REGNO	Other Organization reg. no.
GCMS_FILENAME	Gas chromatograph results
QC_GCMS	Gas chromatography applied?
LOCATION	Room
PLACEMENT	Position within room

The databases are preferably maintained as Oracle relational databases at central station 202. External access to the databases is provided by the Enterprise Server program available from Netscape.

Registry System

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to the present invention. This registration system allows users to register proprietary and commercially available chemical compounds into the chemical compound database. Fig. 3A depicts a top portion 300 of a registration form. Fig. 3B depicts a bottom portion 302 of this registration form. This registration form and the other displays of the interface are preferably stored at central station 202. The web browser at one of remote stations 204 requests the registration form using an HTTP request message. The HTTP request is directed to an address of central station 202 and includes an address (any identification information) of the registration form at central station 202. In response to the HTTP request, central station 202 forwards the registration form to remote station 204 for display. Central Station 202 may dynamically generate the registration form. The registration form is communicated to remote station

204 as an HTML document. This process for presenting a web-based interface may be used for all the user interfaces discussed herein.

The registration form shows locations to enter the fields of Table 2. By selecting a structure area 304, the user invokes a chemical structure drawing tool to designate a two-dimensional chemical structure. By selecting a button 306, the user may reset the contents of the form. To proceed to the next screen of the registration interface, the user selects a registration preview button 308. Once the user selects registration preview button 308, the chemical compound information system compares the entered two-dimensional structure of the compound to the structures of the compounds already stored in the compound database to determine if the new compound has already been registered before.

Fig. 3C depicts an upper portion 310 of a registration preview form. Fig. 3D depicts a lower portion 312 of this registration preview form. The registration preview form includes a message 314 indicating whether or not the molecule is new to the compound database. Upon user selection of a commit button 316, the entered information will be added to the batch database. If the molecule is new, a new record is also added to the compound database.

Also, after the user selects commit button 316, the chemical compound information system displays a registration report form. Fig. 3E depicts an upper portion 318 of this registration report form. Fig. 3F depicts a lower portion 320 of this registration report form. The registration report form confirms the information that has been registered, gives a registration number 322 corresponding to "REGNO", and a time and date 324 of registration.

Operating this registry system over the web is highly beneficial. The user interface is easy to use and can be accessed from any location accessible via the network. In some embodiments, the registry system operates over the Internet permitting registration to occur anywhere in the world.

Background Autonomous Enrichment

Fig. 4 is a top level flowchart describing steps of a background process for enriching the compound database according to one embodiment of the present invention. The background process may operate autonomously without invocation by any user. The

background process sequentially goes through the records of the compound database (step 402) and checks if: (i) the 2 dimensional (2D) structure has been processed (step 404), and (ii) a 3 dimensional (3D) structure, corresponding to the 2D structure, has been added (step 410). If either of these have not been performed the following processes are put into operation depending on which process or processes need to be done.

Preparing the 2D structure preferably involves the application of 2 processes: StripSalt (step 406) and StipProt (step 408) , described below.

StripSalt:

Compounds obtained from commercial suppliers often contain salts which appear in the database as part of the molecule structure; this aids the laboratory chemist but interferes with structure calculations. The program stripsalt identifies disconnected fragments based on the bond connectivity data, and outputs only the largest connected fragment, which is assumed to be the molecule of interest. The technique is given in Fig. 5. It assumes that the structure record contains a list of covalent bonds, each of which connects 2 atoms.

Fig. 5 is a flowchart describing steps of removing disconnected fragments based on bond connectivity data according to one embodiment of the present invention. At step 502, the procedure starts at the first bond. At step 504, the procedure checks whether the both atoms in the bond are without a fragment label. If yes, the procedure assigns a new fragment label to both atom at step 506. If no, the procedure goes to step 508 where it checks whether only one atom in the bond has a fragment label. If yes, the procedure assigns the fragment label of the labeled atom to the unlabeled atom at step 510. If no, the procedure goes to step 512 where it checks if the fragment labels of both atoms are different. If yes, the procedure goes to step 514 where it goes through every atom in the molecule and for those atoms labeled with the same fragment as the second atom in the current bond, it changes the fragment label to match the first atom in the current bond.

Upon a finding of no difference at step 512, and after any one of steps 506, 510, and 514, the procedure checks at step 516 whether the current bond is the last bond. If the current bond is not the last bond, the procedure goes to the next bond at step 518. If the current bond is the next bond, the procedure goes to step 520. At step 520, the

procedure counts the number of atoms in each fragment and outputs only the atoms and bonds in the largest fragment. The smaller fragment is the salt that is removed.

StripProt:

Frequently chemical reagents contain protecting groups which are cleaved during synthesis. It may be preferable to remove them from the database structure. This is important if the structure is used as an input to a database reaction scheme, ensuring that the resulting product structure resembles the actual chemical product. StripProt reads a set of protecting groups as chemical structures from an input file and does a substructure search on the database structure. The input file also contains information about which atoms in the substructure are to be removed when a substructure match is found. The file is an ASCII file which contains a definition of its own format and as such can be modified by the user. The substructure search is an atom by atom mapping algorithm as described in Gluck, D.J. "A Chemical Structure Storage and Search System Developed at Du Pont", J. Chem. Doc. 1965, 5, 43-51, the contents of which are herein incorporated by reference.

Generation and processing of the 3D structure involves 2 main steps: (i) calculation of 3D coordinates (step 414), and (ii) addition of pharmacophoric labels (step 412). The 3D structure is then added to the database. The 3D coordinates are calculated using the Corina program from Oxford Molecular. The pharmacophoric labels are calculated by the program AddPharm, below.

Addpharm:

Identifies pharmacaphoric groups which are relevant to drug design. They are defined as substructures in an input file which are chosen using heuristics about which substructures contain the pharmacophoric groups. For example a carboxylate has a negative charge, aliphatic amine has a positive charge, hydroxyl is both a hydrogen bond donor and acceptor, and so on. The file is an ASCII file which contains a definition of its own format and can be modified by the user. The database structures are searched using the same substructure search algorithm as in StripProt. When there is a substructure hit, the file contains information about which atoms to label with which pharmacophoric type, and these are added as records in the database. The pharmacophoric groups include the following types: A: hydrogen bond acceptor, D:

hydrogen bond donor, H: hydrophobic, N: negatively charged, P: positively charged and R: aromatic. These represent the kinds of interactions observed when a small molecule ligand binds to a protein receptor. A pharmacophore is then a set of such points in a spatial arrangement which represents the interactions made with a particular protein receptor. Therefore the other procedure needed for a full pharmacophore search is a conformation generator; this may be a feature of the database or may be done by an external program.

Fig. 6 depicts a representative compound, sumatriptan succinate. The added pharmacophoric labels are shown. A succinate salt 704 can be seen to be a disconnected fragment and is therefore removed.

Compound Tracking and Acquisition

Fig. 7 is a simplified representation of a laboratory environment where systems and methods according to the present invention may be deployed. A laboratory facility 700 includes a plurality of rooms 702. Each room 702 is preferably equipped with at least one wall-mounted scanner 704 for scanning in chemical compounds. Although, Fig. 7 depicts a single scanner 704 in each room 702, there may be multiple scanners in each room. Any type of data entry device may substitute for the scanners 704. Shelves 706 store containers of chemical compounds. Each depicted room 702 is assumed to be used for experiments or chemical processing. A chemical stock room is not needed. Laboratory facility 700 is merely representative of environments where a compound tracking and acquisition system may be deployed. A compound tracking or acquisition system may be implemented in any physical environment according to the invention.

Fig. 8 depicts details of scanner 704. Scanner 704 includes a scanning wand 802 for reading bar codes from chemical compound containers. Scanning wand 802 is preferably an Intermec 1545 non-contact bar code scanner available from Intermec, Inc. of Everett, Washington. A fixed portion 804 of scanner 704 includes a display 806 for presenting user prompts, a keyboard 808, and an RF unit 810 including an antenna 812. Except for RF unit 810 and antenna 812, fixed portion 804 may be a 9560 transaction manager available from Intermec.

In one scenario, when a container arrives in a facility receiving department, a preprinted barcode label is affixed to the outer packaging. A single box including many containers may have several labels. The containers are then initially registered in the database on central station 202. The containers are delivered to individual rooms 702 where the bar codes are scanned in. Whenever a container moves it is rescanned.

Fig. 9 is a flowchart describing steps of registering a new location for a chemical compound container according to one embodiment of the present invention. At step 902, a user waves wand 802 over a bar code on a chemical container. Once the bar code has been read, RF unit 810 transmits the new location information to central station 702 at step 906. RF unit 810 preferably operates around 800 MHz. Central station 202 is similarly equipped with RF receiver equipment (not shown). At step 908, central station 202 modifies the container location information in its database. Preferably, the DataConnect program available from Connectware, Inc. of Santa Clara, California interfaces between the scanner system and the databases described above.

Optionally, a user may register consumption of compound even without change of location by scanning the bar code and making appropriate entries on keyboard 808. The user may also similarly register complete depletion of the bottle contents and automatically reorder fresh stock.

Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention. Fig. 10 will be described with reference to Figs. 11A-11F which illustrate a user interface for acquiring a chemical compound. An advantage provided by virtue of the present invention is the ability to use an interface both for searching for a compound internally, and for acquiring the compound from an external source. The user interface is assumed to be active at one of remote stations 204, although it would of course be also possible to operate it at central station 202. In a preferred embodiment, the interface is web-based.

At step 1002, the user enters search criteria giving characteristics of the desired compound. Fig. 11A depicts the user interface for this step. The user may enter a chemical name or a chemical formula. Other textual or numerical criteria include the amount of chemical compound desired, the registration number, the catalog number or the location.

The user may also enter the structure in a structure area 1102 to find a compound having the same or similar structure to the entered structure. The user may also use structure area 1102 specify a substructure that would be found within the desired compound. The user may also specify a configuration of pharmacaphoric groupings that can be presented by the compound as shown in Fig. 12. Fig. 12 depicts that an acceptor 1202, donor 1204, and aromatic 1206 are presented. To meet the bonding criterion determined by the depicted configuration, a compound must be able to present these pharmacaphoric groupings at the spacings indicated in Fig. 12. A pull-down menu 1104 is used to select among these various types of structural criteria.

At step 1004, central station 202 searches for compounds having the desired characteristics in the compound database and the batch database. At step 1006, remote station 204 displays the structures of compounds having characteristics matching the search criteria. A representative display for this step is depicted in Fig. 11B. For each compound the display shows a structure 1106, a registration number 1108 for the compound. When the compound is available internally, one or more location codes are also shown. When the compound is available externally, the number of suppliers 1110 is shown. Fig. 11C depicts an alternative view of the search results where more information is depicted including a molecule name 1112, a molecular formula 1114, and a molecular weight 1116.

At step 1008, by clicking on any displayed location code, the user can call up a display of a site map which the user may refer to find the physical location of the desired compound. Fig. 11D shows such a site map display 1118. In an alternative embodiment, the display may show a special icon at the location of the compound, or may show directions to the location of the compound from the user's location.

At step 1010, by clicking on the number of suppliers 1110, the user may call up a catalog display 1120 as shown in Fig. 11E. Catalog display 1120 lists vendors, and for each vendor, catalog entries for compounds satisfying the search criteria. For each catalog entry, the display may further include a purity percentage, an indicator of quantity per batch, and a price. The user may specify a desired quantity in one of quantity boxes 1122 and specify a particular catalog entry for order by clicking in one of "add to cart" boxes 1124. When the user is ready to add all of the desired catalog entries to a "virtual shopping cart," the user selects an add to cart button 1126.

Fig. 11F depicts a virtual shopping cart 1128 that lists desired compounds and their previously selected sources. Virtual shopping cart 1128 is displayed at step 1012. A current total price 1130 is given. The user can place an order for the selected items by selecting a place order button 1132. The user can also name the cart for future reference by selecting a name this cart button 1134, clear the cart by selecting a clear cart button 1136, or select a new cart by selecting a new cart button 1138. In one embodiment, when the user selects the cart, the orders are sent to a purchasing department. In another embodiment, when the user selects the cart, the orders are sent directly to the suppliers over the Internet. Payment information may be included with the electronic orders.

The result is a virtual inventory system that allows users to obtain desired compounds quickly and efficiently from both internal and external sources. Benefits include lower cost acquisition since compounds are only requested if they are not available internally, savings in search manpower, and better tracking of costs.

In the foregoing specification, the invention has been described with reference to specific exemplary embodiments thereof. It will, however, be evident that various modifications and changes may be made thereunto without departing from the broader spirit and scope of the invention as set forth in the appended claims and their full scope of equivalents. For example, in any depicted flowcharts, steps may be deleted, substituted, or reordered within the scope of the present invention. Any user interface depicted as being web-based may also be implemented locally, or using any network protocol. For web-based implementations, links may be provided among any combination of the user interface displays to permit free navigation.

WHAT IS CLAIMED IS:

1. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously invoking a three-dimensional structure evaluation routine to determine a three-dimensional structure of said compound based on said two-dimensional chemical structure as a part of said background database management process.

2. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove salts from said two-dimensional chemical structure.

3. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove protective groups from said two-dimensional chemical structure.

4. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database and 3D structures;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said 3D-dimensional chemical structure to identify pharmacaphores in said 3D-dimensional chemical structure.

5. A computer-implemented method for facilitating acquisition of chemical compounds comprising the steps of:

operating an available compound database identifying chemical compounds available within an organization;

accepting user input identifying a desired chemical compound;

searching for said desired chemical compound within said available compound database; and

presenting information concerning availability of said desired chemical compound within said organization and availability from at least one external source.

6. The system of claim 5 wherein said database comprises a plurality of records, each record associated with a particular chemical compound container and indicating a last known location of said chemical compound container.

7. A computer-implemented method for procuring a desired chemical compound comprising:

a) accepting user input indicating a desired chemical compound;

b) searching for one or more container holding said desired chemical compound in a first database, said first database listing available chemical compound containers and their locations; and

c) if no container holding said desired chemical is found in said b) step, searching a second database for said desired chemical compound, said second database storing ordering information for a plurality of chemical compounds.

8. The method of claim 7 wherein said user input comprises a name of said desired chemical compound.

9. The method of claim 7 wherein said user input comprises a chemical structure of said desired chemical compound.

10. The method of claim 7 wherein said user input comprises a chemical substructure found within said desired chemical compound.

11. The method of claim 7 wherein said user input comprises a chemical structure similar to a chemical structure of said desired chemical compound.

12. The method of claim 7 further comprising:

if any container of said desired chemical compound is found in said first database, displaying a location of said container.

13. The method of claim 7 further comprising:

if said desired chemical compound is found in said second database, displaying ordering information for said desired compound.

14. The method of claim 13 further comprising:

accepting user input ordering said desired compound; and

relaying said user input ordering said desired compound to a chemical compound source via a network.

15. A computer-implemented method for registering a chemical compound to a remote database comprising:

accepting user input at a local client specifying an address of a compound input form at a remote server;

in response to said user input, sending a request for said compound input form to said remote server;

in response to said request, transferring data representing said compound input form from said remote server to said local client;

based on said data, displaying said compound input form at said local client, said compound input form including fields for holding compound characteristics;

accepting user input at said local client specifying contents of one or more of said field;

forwarding said contents from said local client to said remote server; and

adding said contents to a compound database accessible by said remote server.

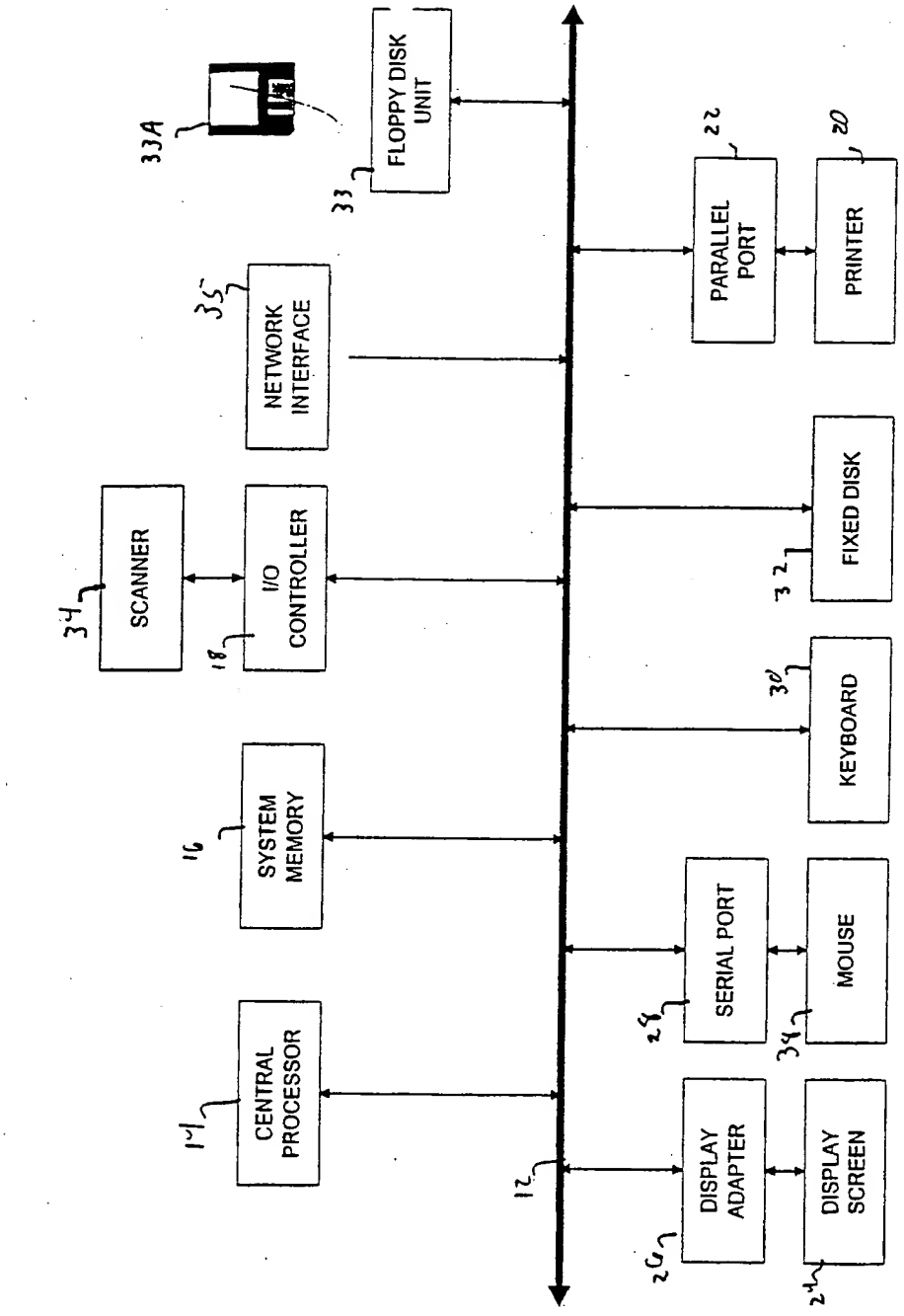
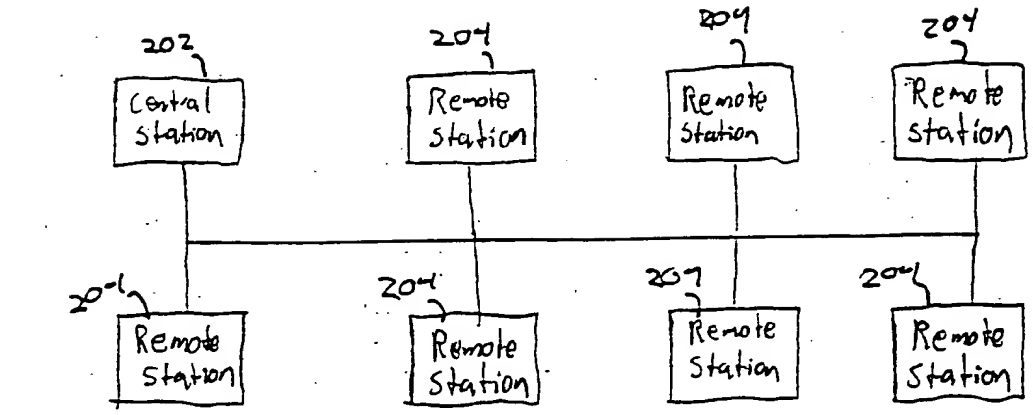


Fig. 1


200
202
Central Station
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Remote Station
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Remote Station
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204
Remote Station

Fig. 2

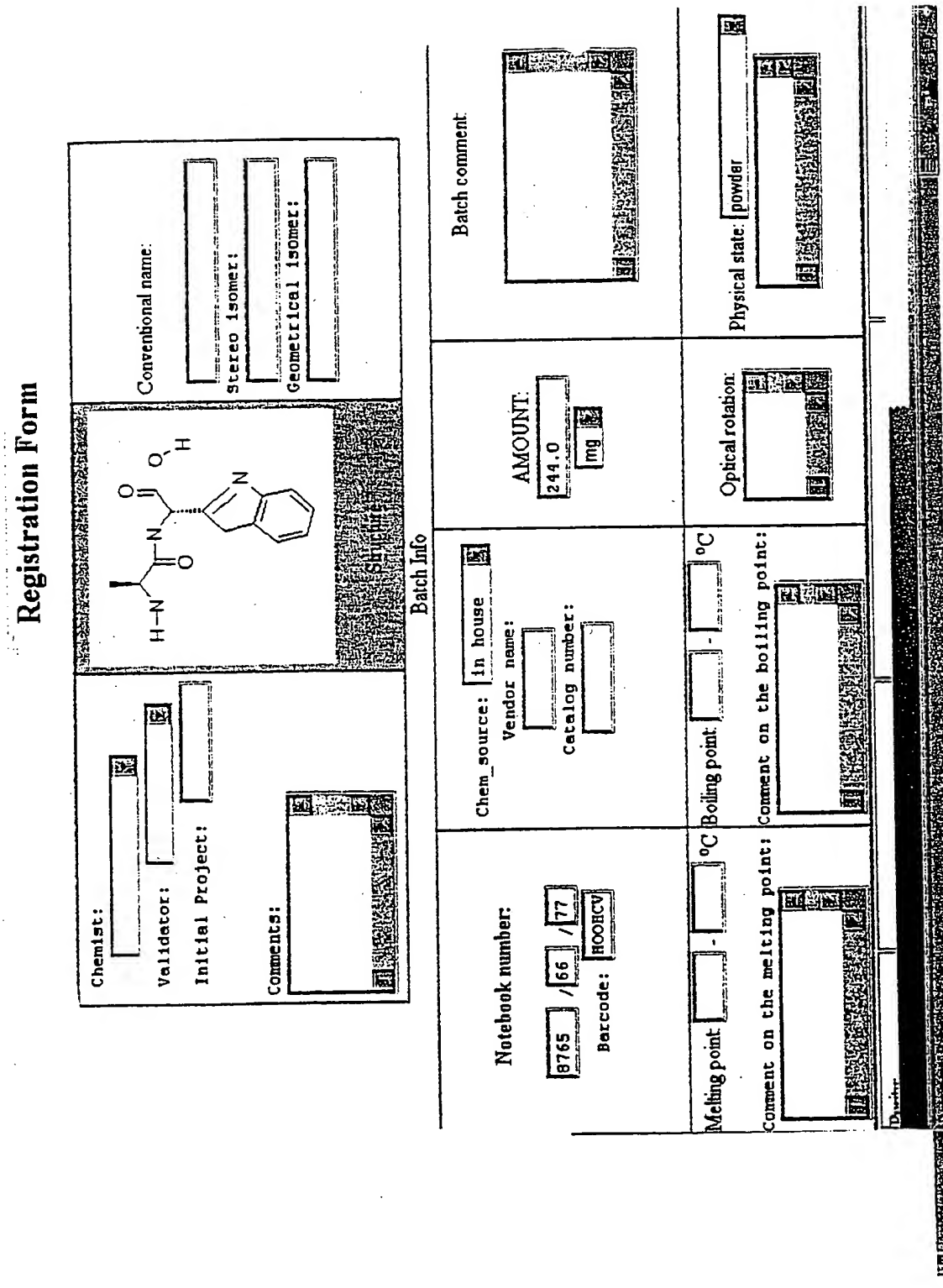
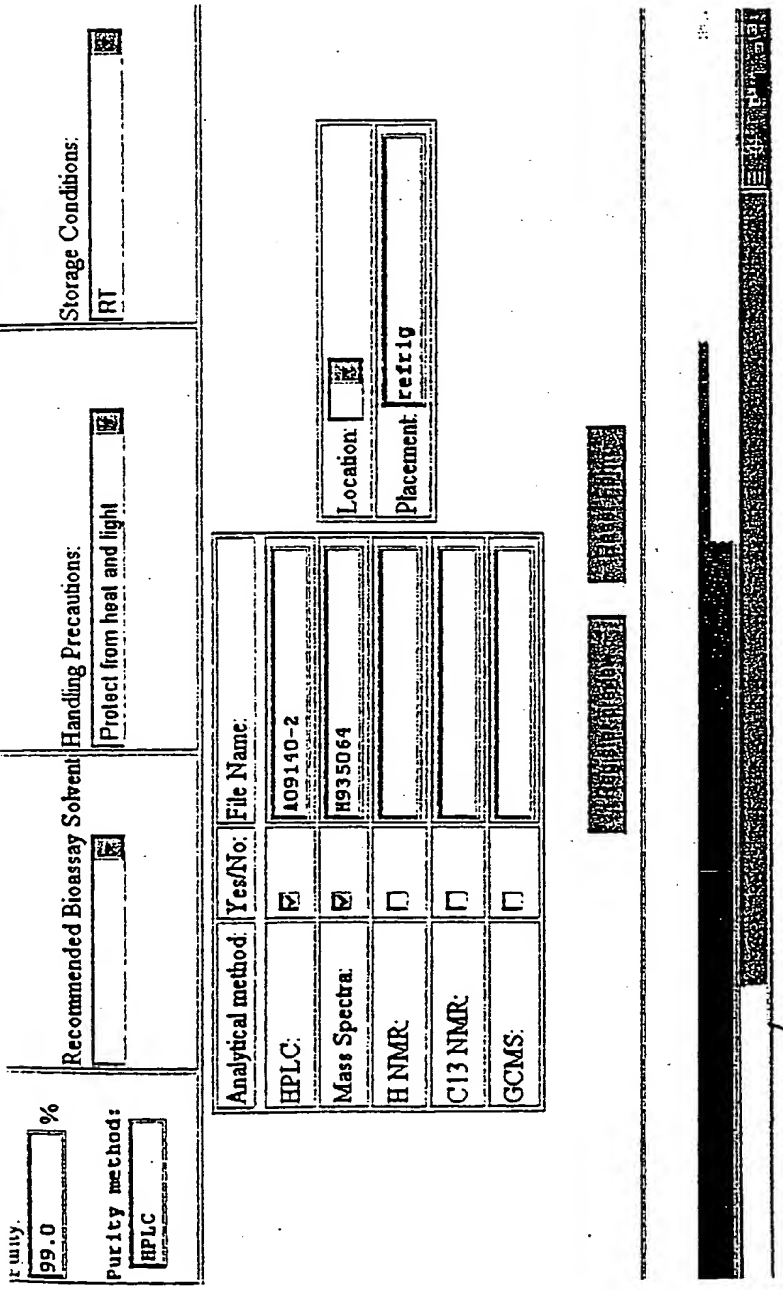


FIG. 3A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RT
Handling Precautions:
Protect from heat and light
Recommended Bioassay Solvent:
Location:
Placement:
refrig
Analytical method:
Yes/No:
File Name:
HPLC:
409140-2
Mass Spectra:
H9350G4
H NMR:
C13 NMR:
GCMS:
Purity method:
HPLC
99.0
%
32

Fig. 3B

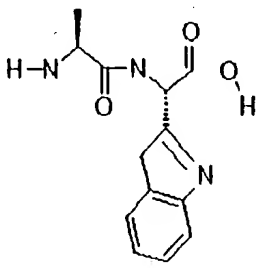
Registration Preview Form

The molecule is new to the database.

The structure and batchinfo will be registered if you commit.

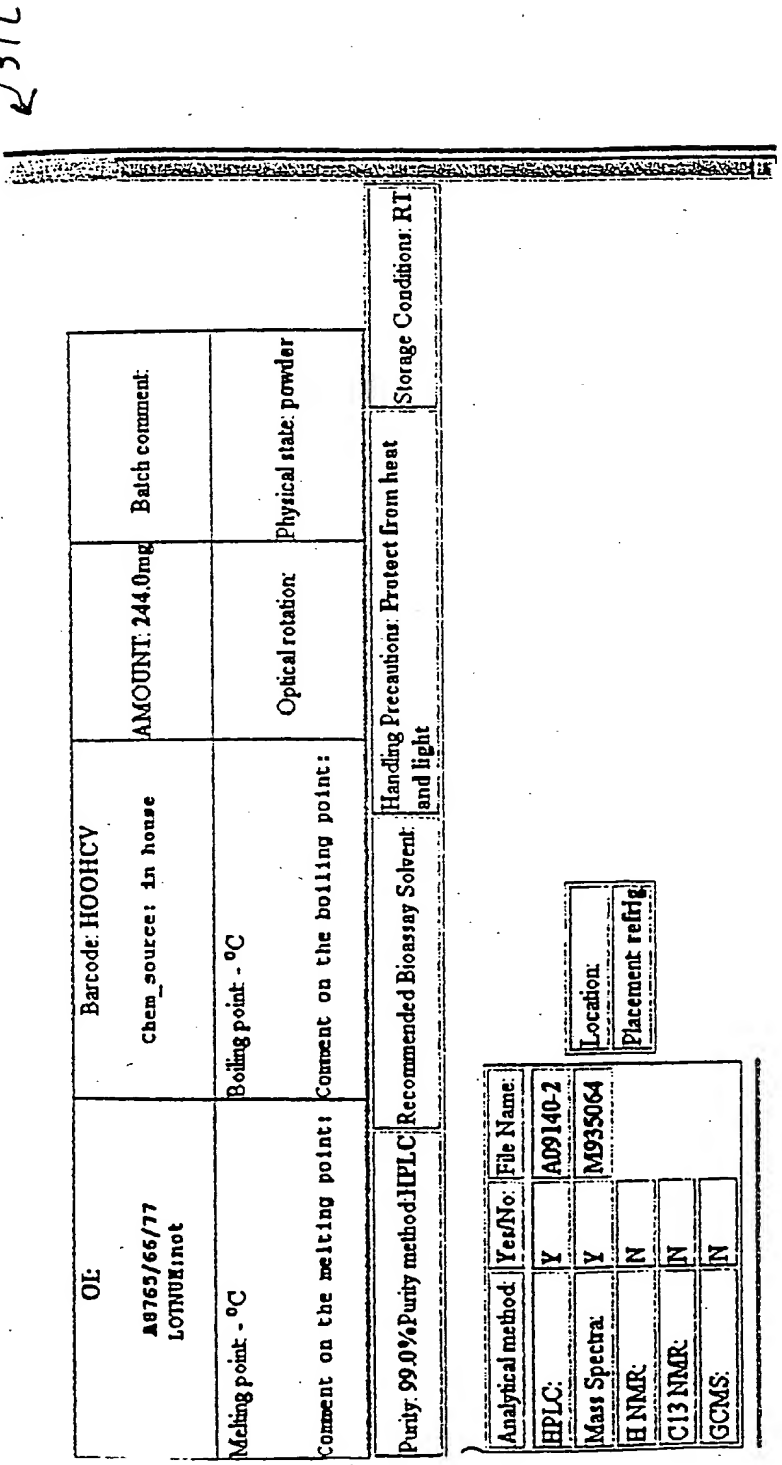
[redacted] 314

ChemBank sample info:

Mol regno number is :		Conventional name:
no info Chemist: Charlie Peng Validator: Steve Muskal Initial Project: Molecular Weight: not calculated yet Molecular Formula: not calculated yet	 Structure	Stereo isomer: Geometrical isomer: Comments:

310

Fig. 3C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A8765/66/77
LOTNUM:not
Barcode: HOOHCV
Chem_source: in house
AMOUNT: 244.0mg
Batch comment:
Melting point - °C
Boiling point - °C
Optical rotation:
Physical state: powder
Comment on the melting point:
Comment on the boiling point:
Purity: 99.0%Purity method:HPLC
Recommended Bioassay Solvent:
Handling Precautions: Protect from heat and light
Storage Conditions: RT
Analytical method
Yes/No
File Name
HPLC:
Y
A09140-2
Mass Spectra:
Y
M935064
H NMR:
N
C13 NMR:
N
GCMS:
N
Location:
Placement refrig

Fig. 3D

ChemBank Registration Report Form

324

month [redacted] date [redacted] year [redacted] time : [redacted]

322

Your assigned compound registration number is : CB10093

ChemBank sample info:

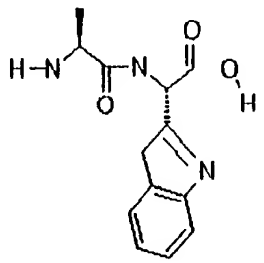
AF number is : CB10093 Chemist: Charlie PengInitial Project: null Validator: Steve Huskal Molecular Weight: Molecular Formula:	 Structure	Conventional name: Stereo isomer: Geometrical isomer: Comments:

Fig. 3E

OI: A8765/66/77 LOTNUM:1	Barcode: HOOHCV Chem_source: in house	AMOUNT: 244mg	Batch comment: null
Melting point: 0-0 °C Comment on the melting point:	Boiling point: 0-0 °C Comment on the boiling point:	Optical rotation:	Physical state: powder

Purity: 99% Purity method: HPLC	Recommended Bioassay Solvent: null	Handling Precautions: Protect from heat and light	Storage Conditions: RT

Analytical method:	Yes/No:	File Name:
HPLC:	Y	A09140-2
Mass Spectra:	Y	M935064
H NMR:	N	
C13 NMR:	N	
GCMS:	N	

Location: null
Placement: refrig

320

Fig. 3F

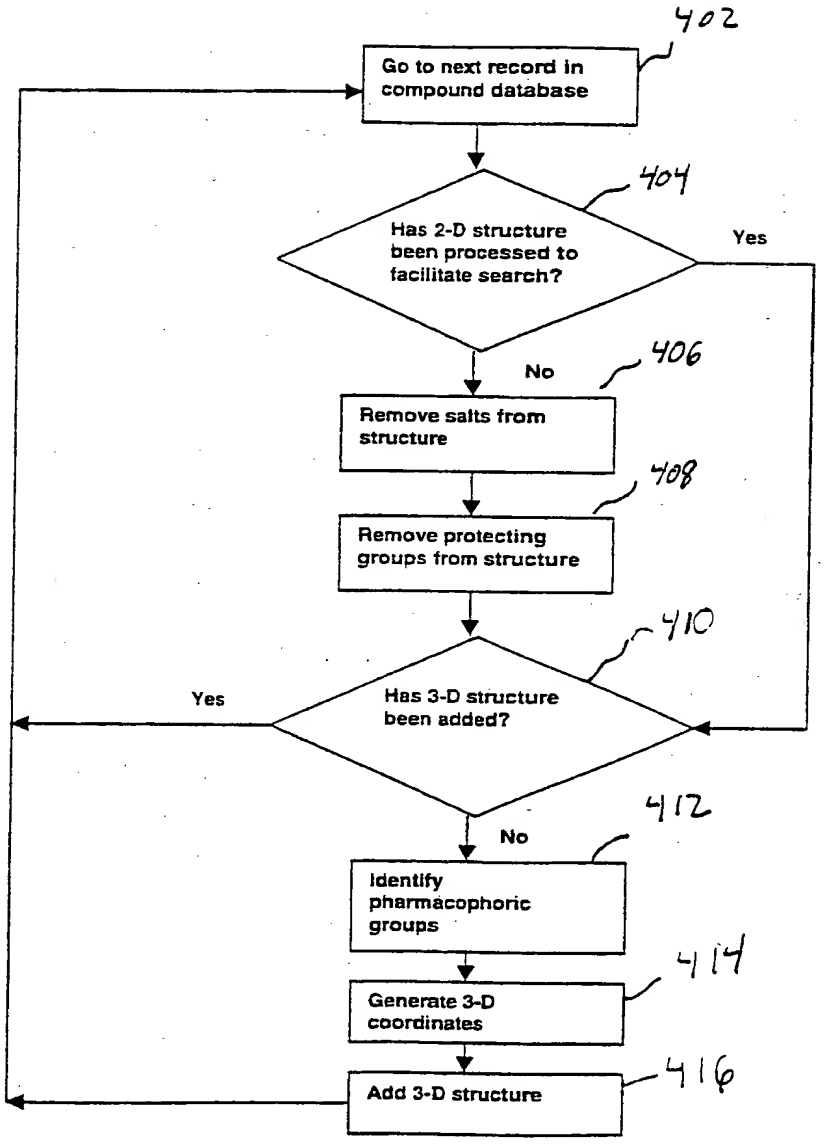


Figure 4

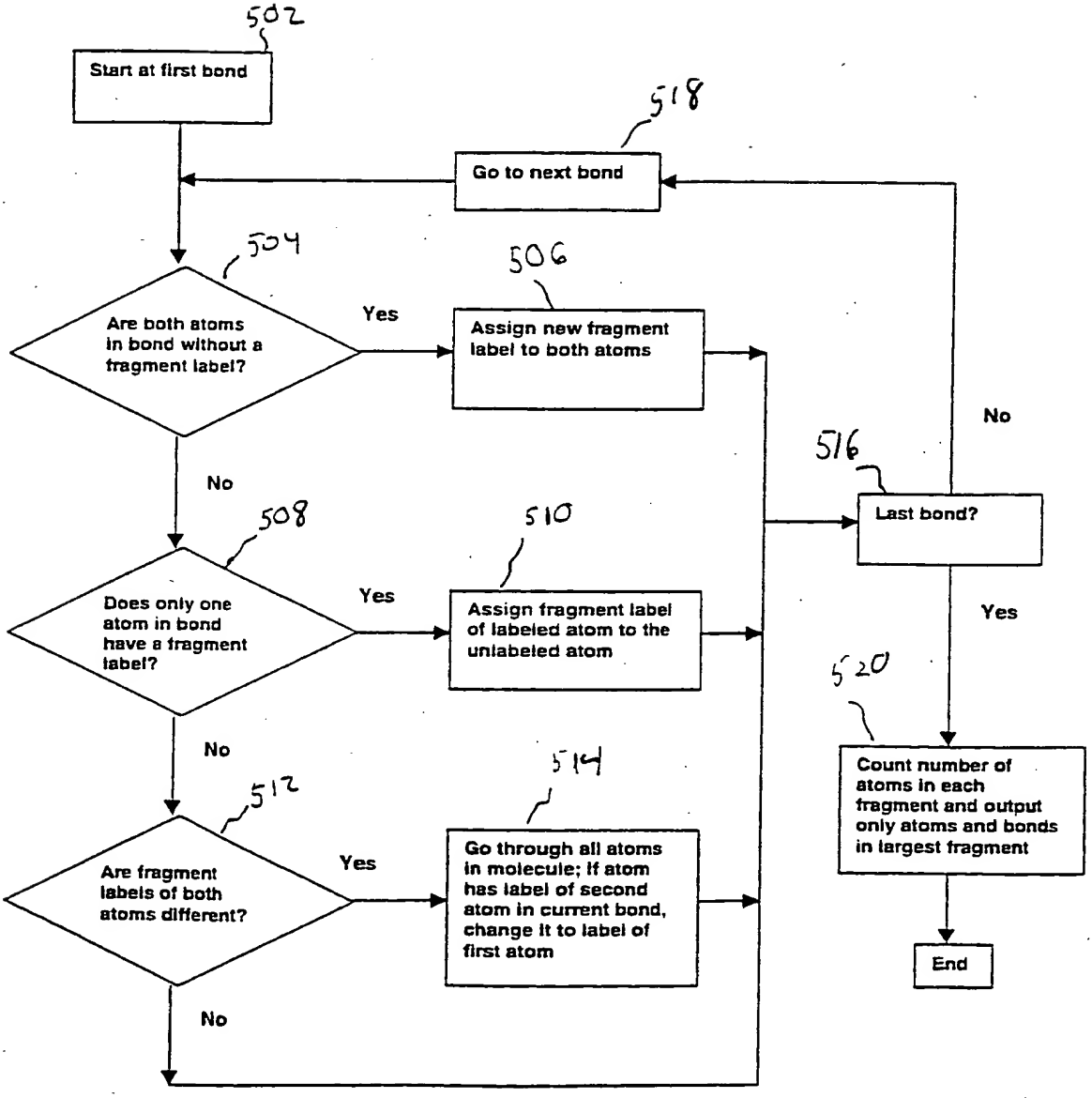
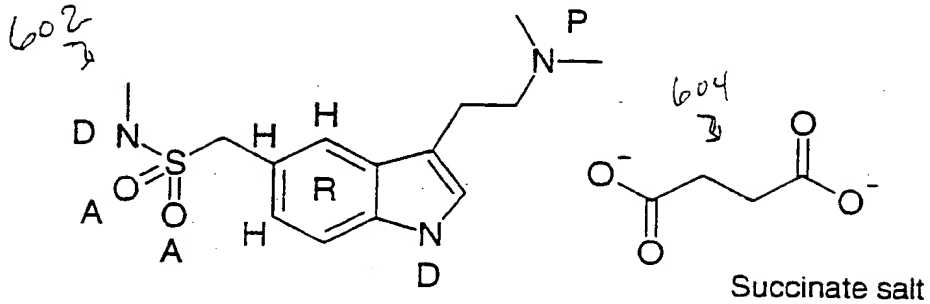

502
Start at first bond
518
Go to next bond
504
Are both atoms in bond without a fragment label?
Yes
506
Assign new fragment label to both atoms
No
516
Last bond?
No
Yes
508
Does only one atom in bond have a fragment label?
Yes
510
Assign fragment label of labeled atom to the unlabeled atom
No
520
Count number of atoms in each fragment and output only atoms and bonds in largest fragment
512
Are fragment labels of both atoms different?
Yes
514
Go through all atoms in molecule; if atom has label of second atom in current bond, change it to label of first atom
No
End

Figure 5

Sumatriptan succinate



Succinate salt (removed)

Pharmacophore labels added:
A : hydrogen bond acceptor
D : hydrogen bond donor
H : hydrophobic
N : negative charge
P : positive charge
R : aromatic

Fig. 6

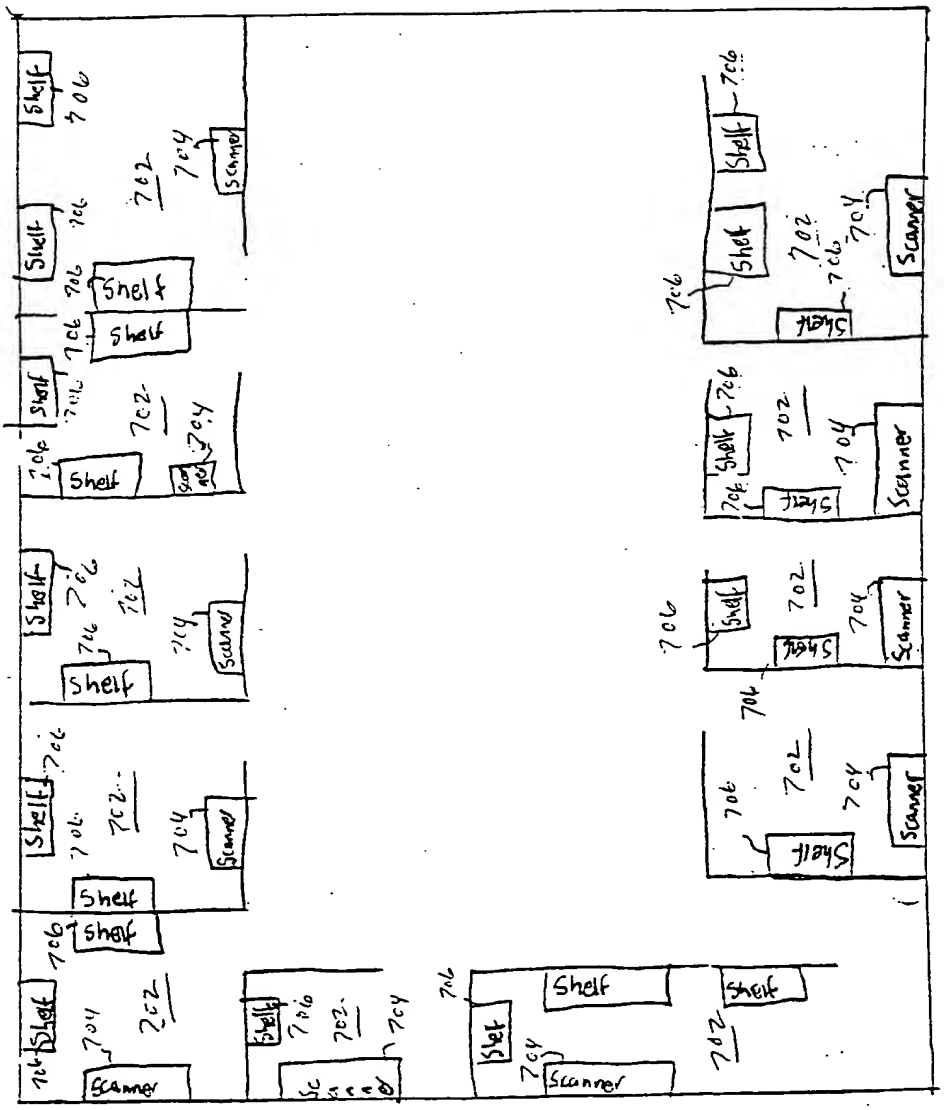


Fig. 7

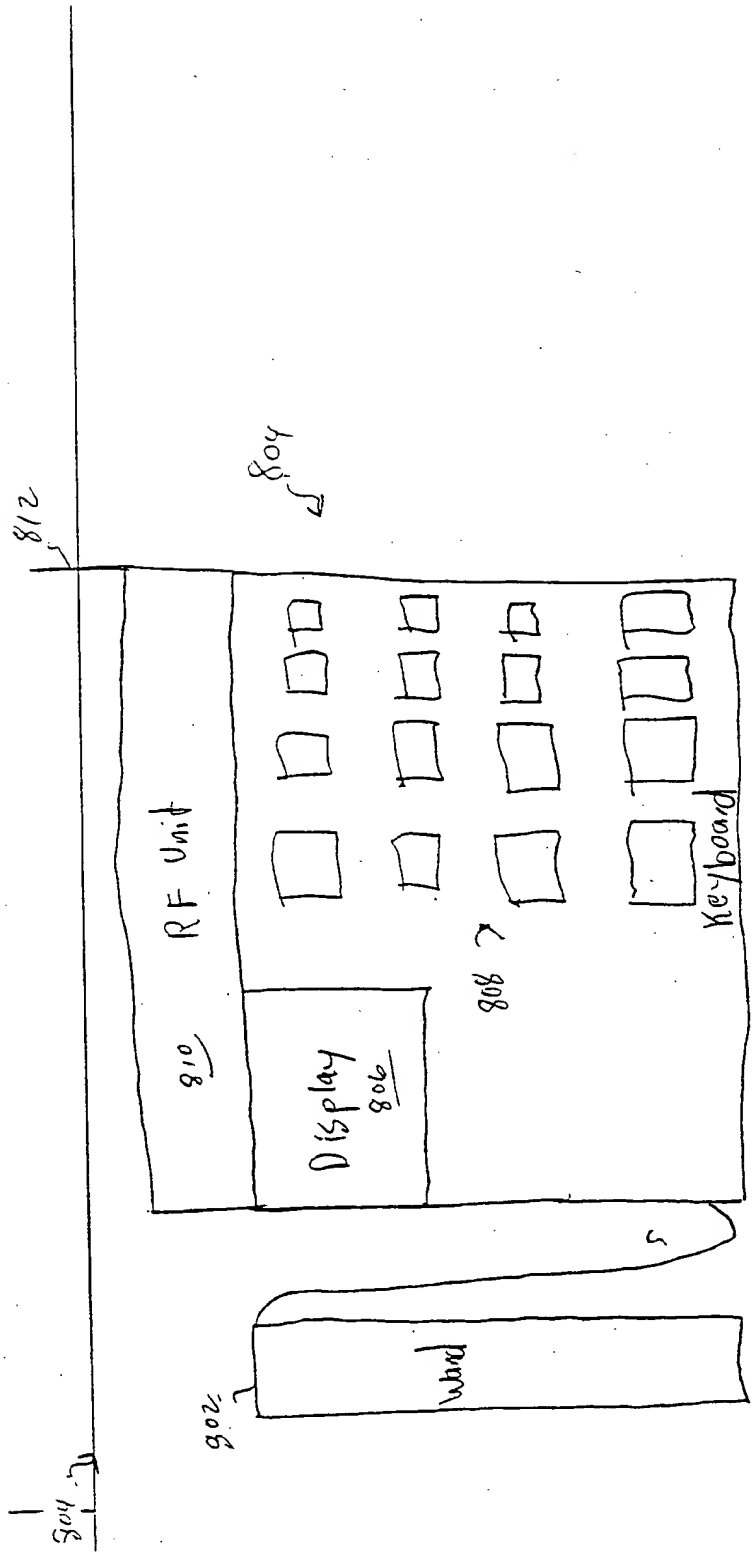
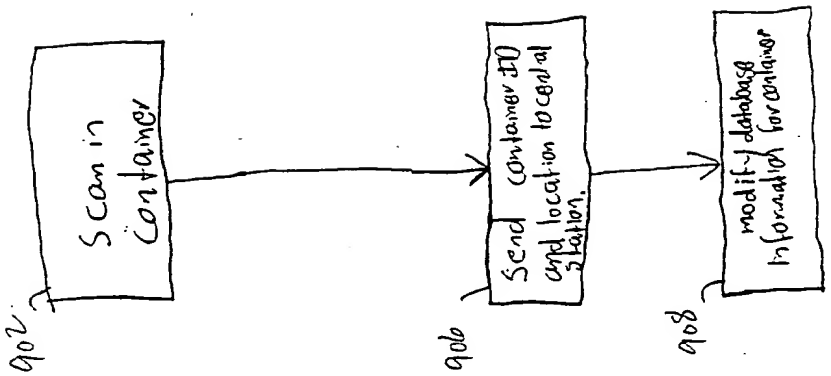


Fig. 8



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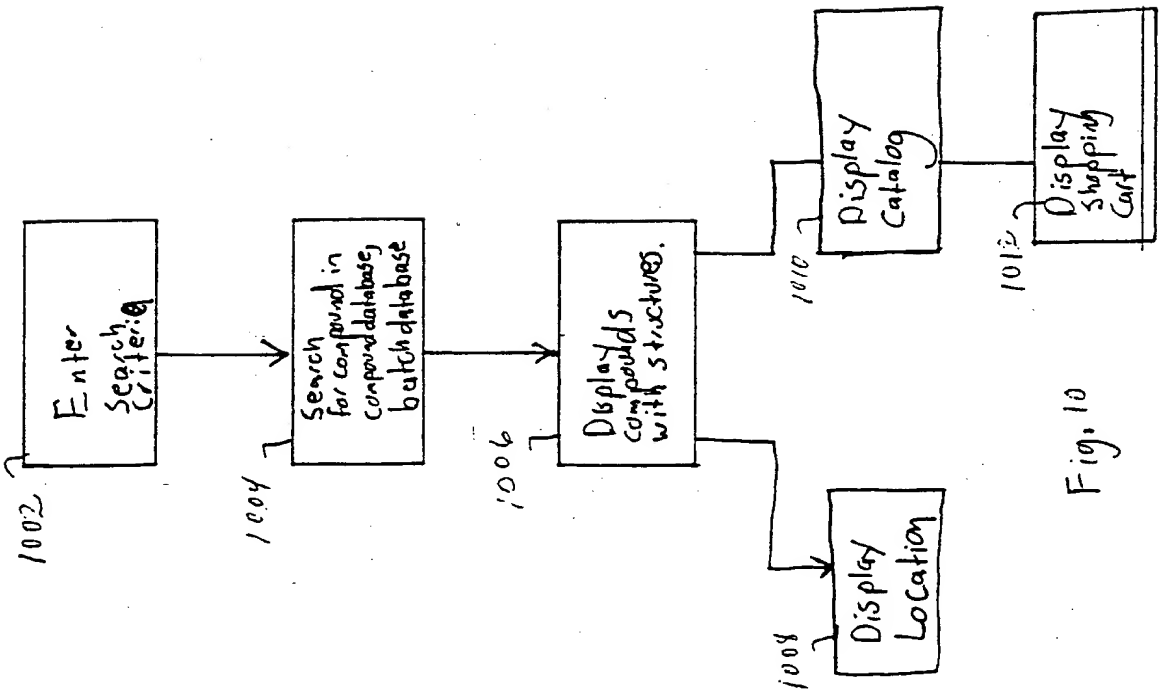
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1006
Display Catalog
1010
Display Shopping Cart
1012
Display Location
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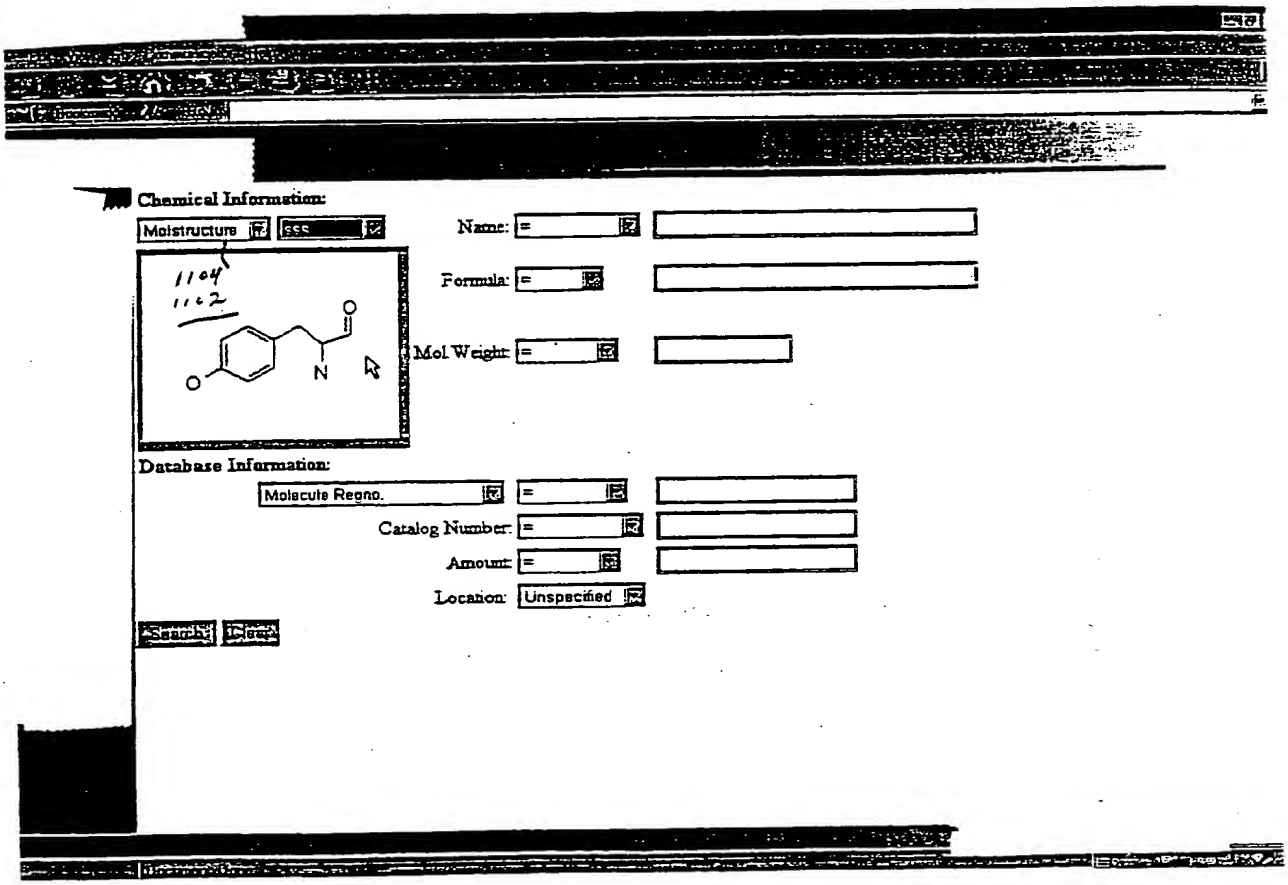
Fig. 10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Name:
Formula:
Mol Weight:
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Catalog Number:
Amount:
Location:
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Search
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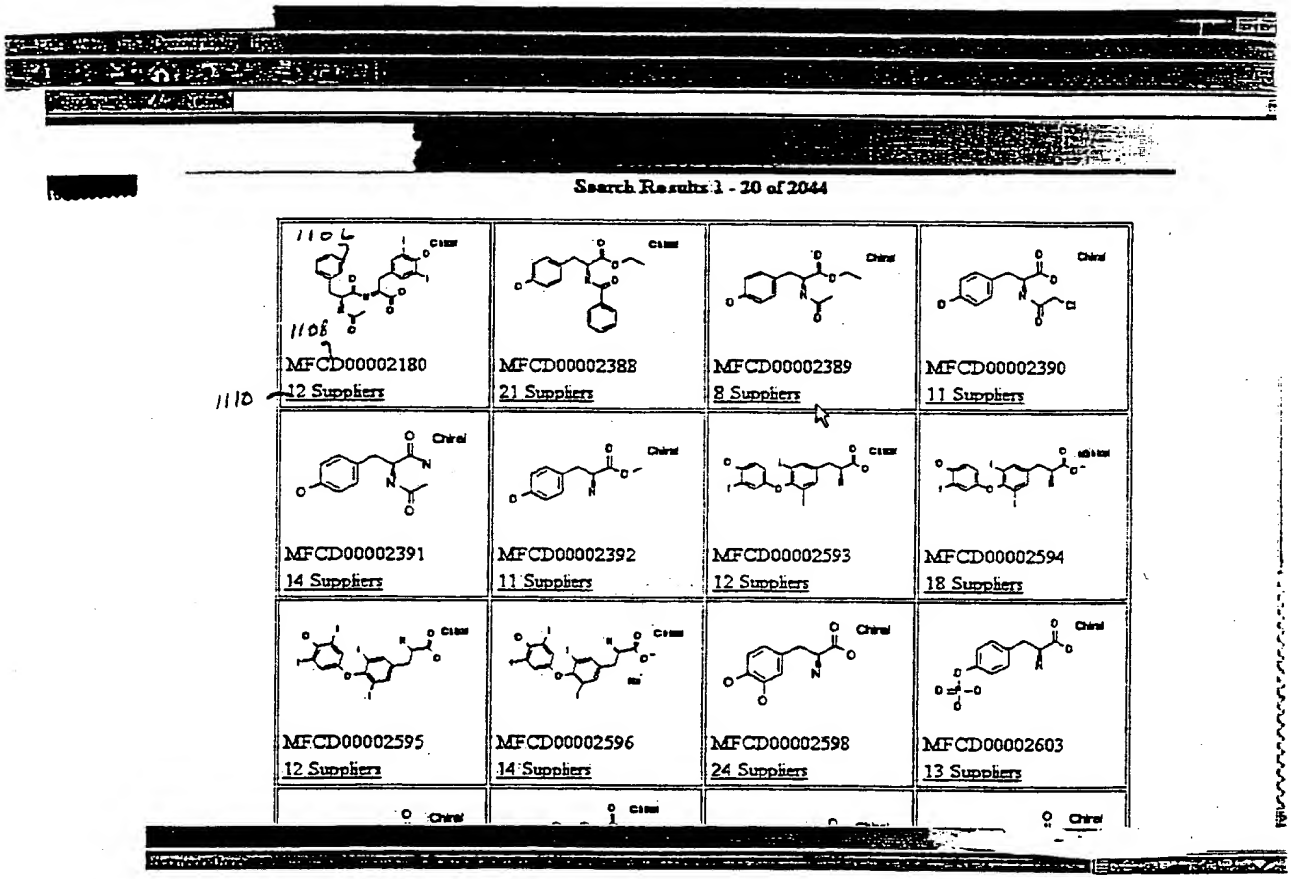
Fig. 11A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1110
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12 Suppliers
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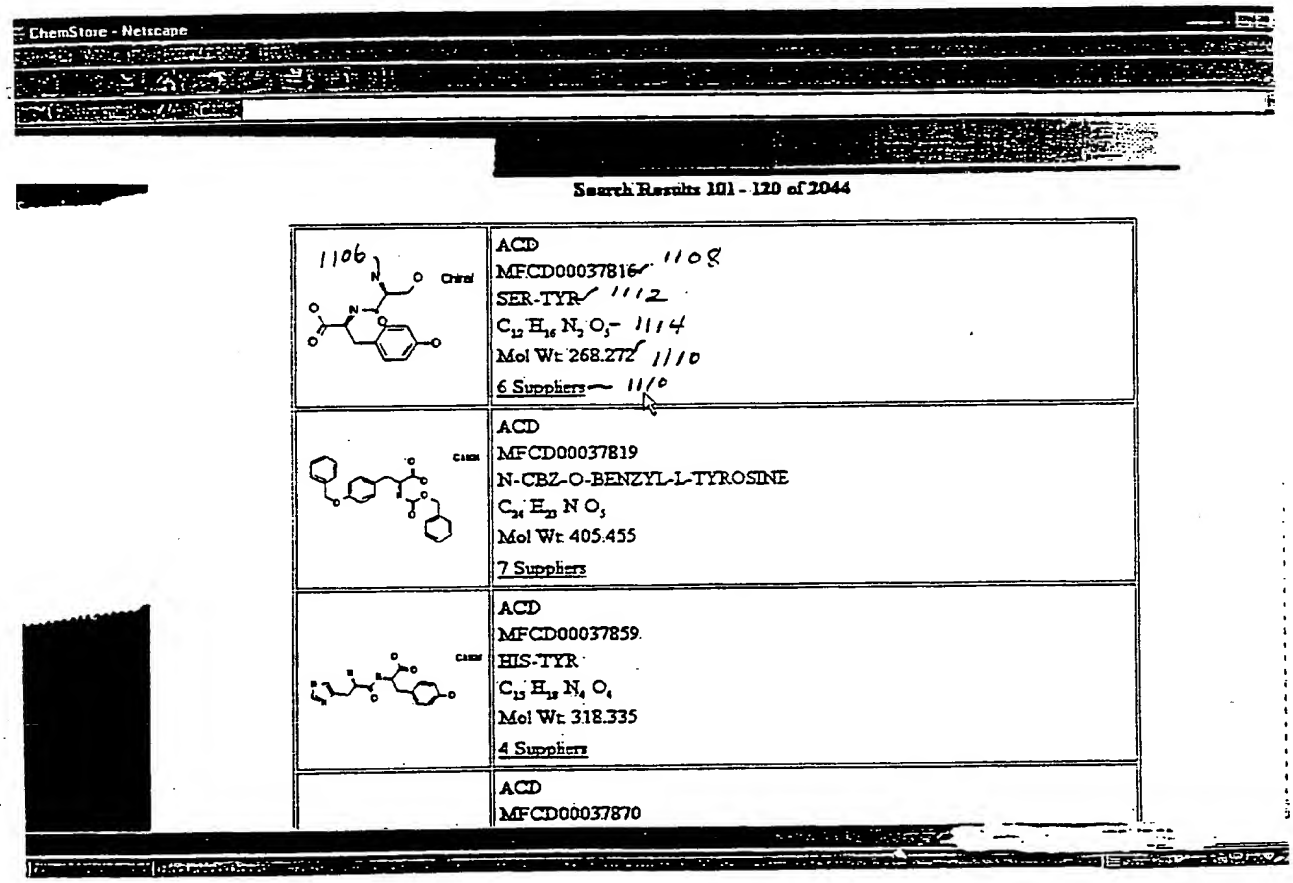
MFCD00002603
13 Suppliers

Fig. 11B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Search Results 101 - 120 of 2044
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6 Suppliers 1110
ACD
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$C_{24}H_{23}NO_5$
Mol Wt 405.455
7 Suppliers
ACD
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$C_{15}H_{18}N_4O_4$
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Fig. 11c

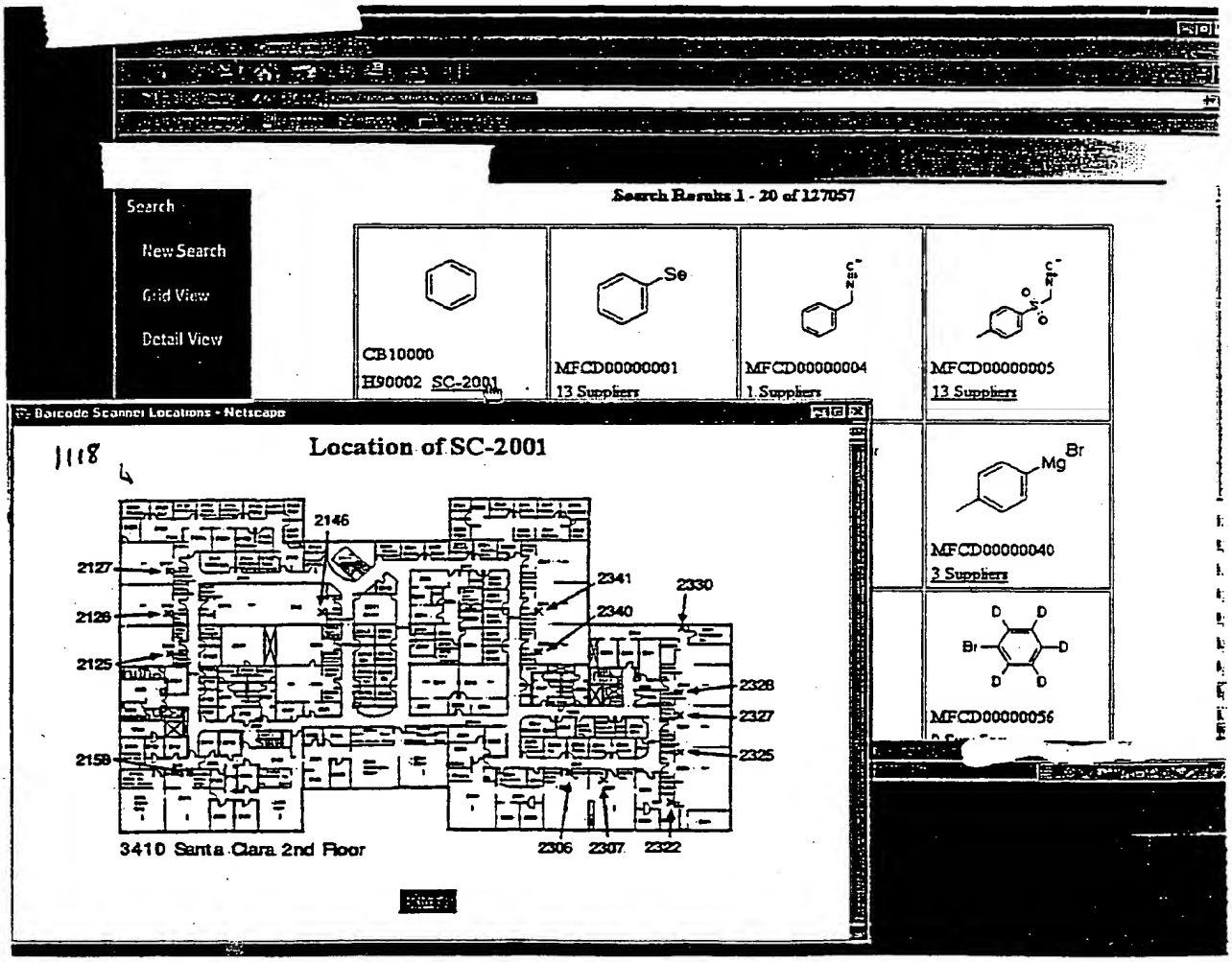
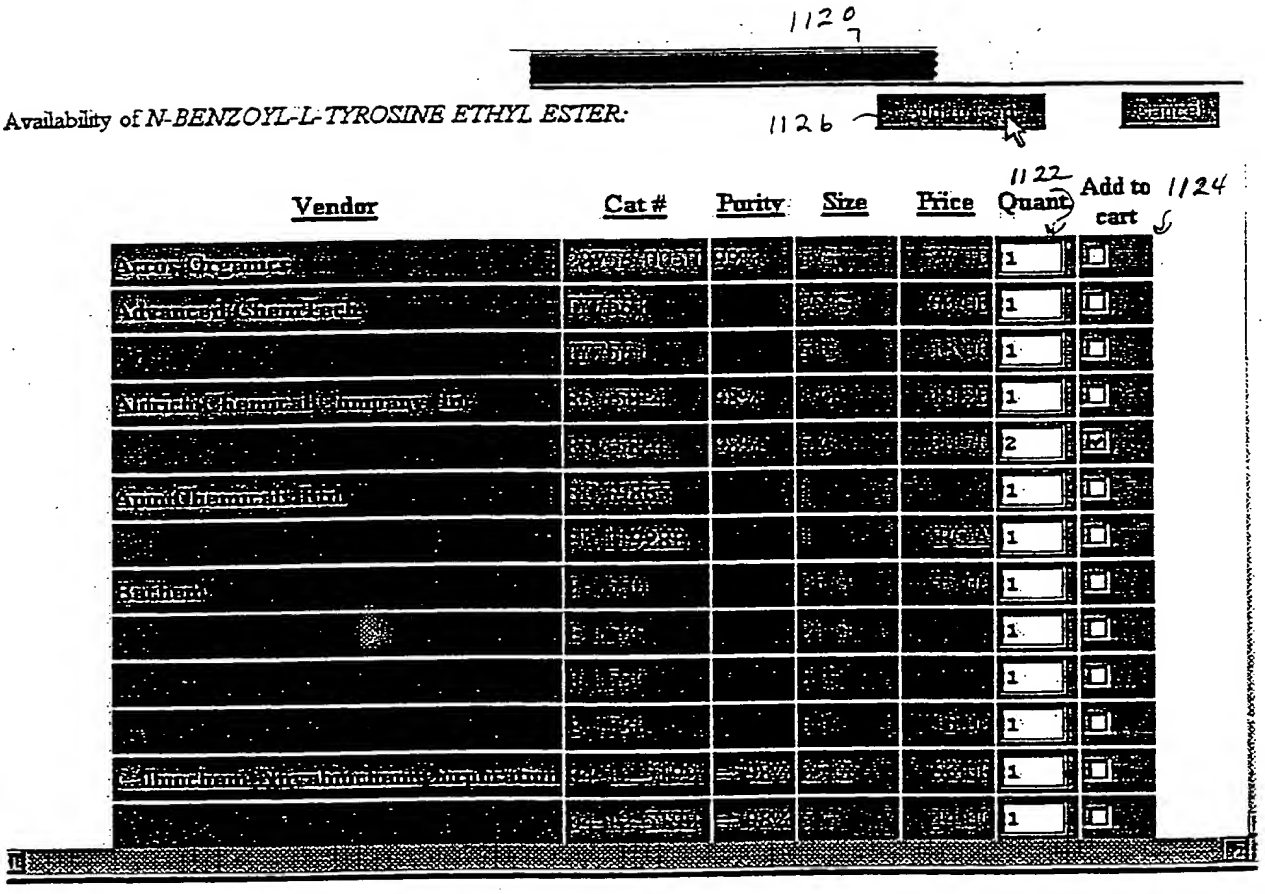


Fig. 11D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1126
Cancel
1122
Vendor
Cat #
Purity
Size
Price
Quant
Add to cart
1124

Fig. 11E

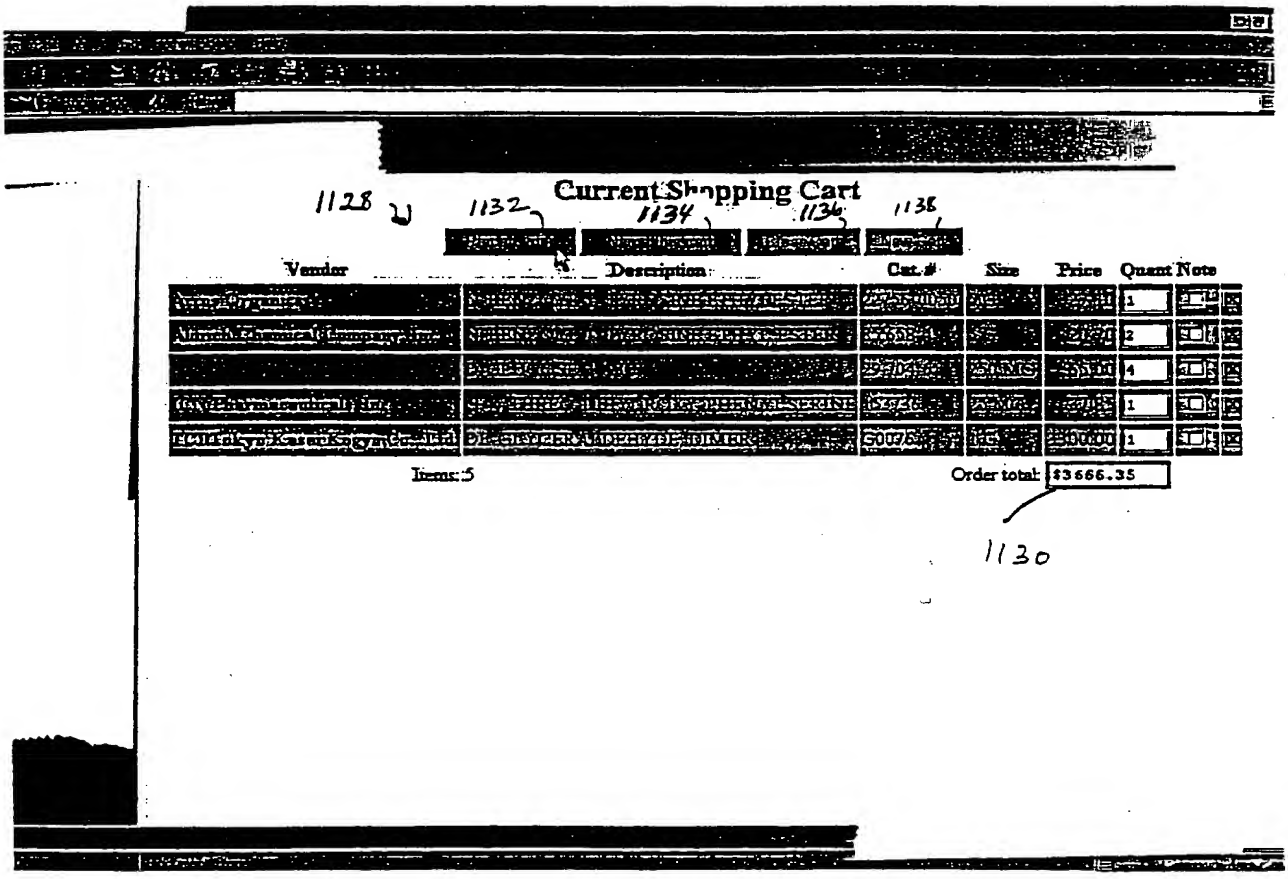


Fig. 11F

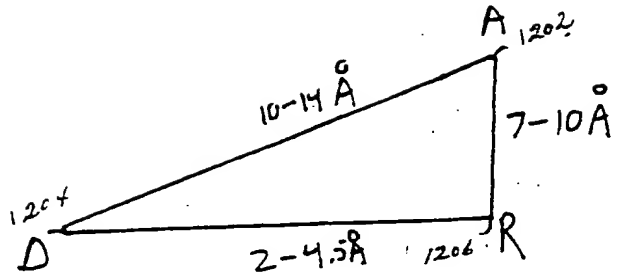


Fig. 12

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US99/15688

A. CLASSIFICATION OF SUBJECT MATTER
IPC(6) :G06F 17/30
US CL :707/1, 100
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 707/1, 100, 3

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

APS, CAS ONLINE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	US 5,577,239 A [MOORE ET AL.] 19 NOVEMBER 1996, SEE ABSTRACT	1-15
Y	US 5,321,804 A [KUSABA ET AL.] 14 JUNE 1994, SEE ABSTRACT	1-15
A, P,	US 5,787,279 A [RIGOUTSOS] 28 JULY 1998, SEE ABSTRACT	1
A	US 5,418,944 A [DIPACE ET AL.] 23 MAY 1995, SEE ENTIRE DOCUMENT	1
A, P	US 5,812,134 A [POOSER ET AL] 22 SEPTEMBER 1998, SEE ABSTRACT.	1

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

*	Special categories of cited documents:	"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"A"	document defining the general state of the art which is not considered to be of particular relevance	"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"E"	earlier document published on or after the international filing date	"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"&"	document member of the same patent family
"O"	document referring to an oral disclosure, use, exhibition or other means		
"P"	document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 27 AUGUST 1999	Date of mailing of the international search report 28 OCT 1999
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230	Authorized officer SANJIV SHAH Telephone No. (703) 305-8355

Form PCT/ISA/210 (second sheet)(July 1992) ★

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

CORRECTED VERSION

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
20 January 2000 (20.01.2000)

PCT

(10) International Publication Number
WO 00/03336 A1

(51) International Patent Classification[6]: G06F 17/30

(21) International Application Number: PCT/US99/15688

(22) International Filing Date: 12 July 1999 (12.07.1999)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
09/114,694 13 July 1998 (13.07.1998) US

(63) Related by continuation (CON) or continuation-in-part (CIP) to earlier application:
US 09/114,694 (CIP)
Filed on 13 July 1998 (13.07.1998)

(71) Applicant *(for all designated States except US)*: GLAXO GROUP LIMITED [GB/GB]; Glaxo Wellcome House, Berkeley Avenue, Greenford, Middlesex UB6 0NN (GB).

(72) Inventors; and

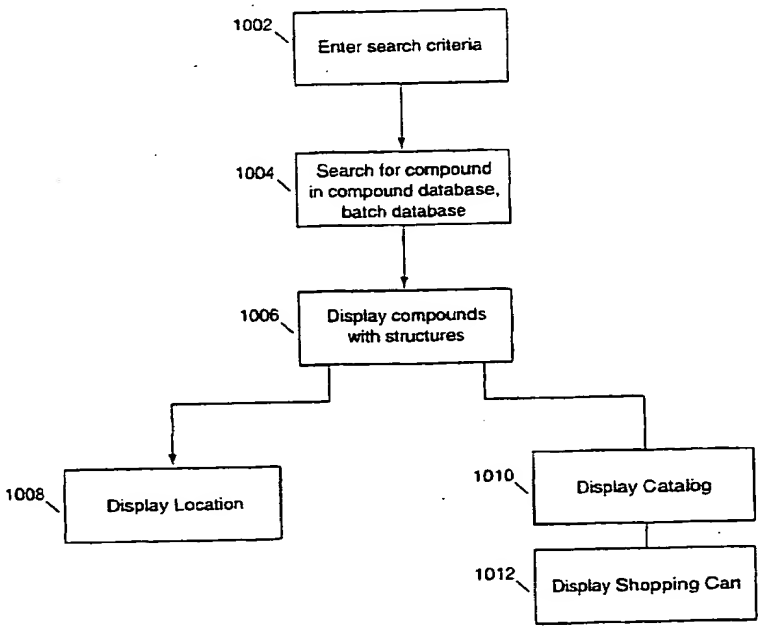
(75) Inventors/Applicants *(for US only)*: MUSKAL, Steven, Marc [US/US]; 2656 Hesselbein Way, San Jose, CA 95148 (US). EGLI, Paul, Andrew [US/US]; 39865 Cedar Boulevard #342, Newark, CA 94560 (US). PENG, Chunyang [CN/US]; 20650 Park Circle E. #1, Cupertino, CA 95014 (US). MCGREGOR, Malcolm, James [GB/US]; 655 S. Fair Oaks Avenue #G302, Sunnyvale, CA 94086 (US).

(74) Agent: STEVENS, Lauren, L.; Affymax Research Institute, 4001 Miranda Avenue, Palo Alto, CA 94304 (US).

(81) Designated States *(national)*: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW.

[Continued on next page]

(54) Title: CHEMICAL COMPOUND INFORMATION SYSTEM



(57) Abstract: Systems and methods for managing chemical compound information. Chemical compound tracking and purchasing systems may be provided. A user interface (1002) allows for queries to identify compounds (1004) available internally to the organization and for orders from external sources for compounds that are unavailable internally. Background processing of compound characteristics as stored in a chemical compound database (1004) may be provided (1006).

WO 00/03336 A1

(84) **Designated States** *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *With international search report.*

(48) **Date of publication of this corrected version:**
15 February 2001

(15) **Information about Correction:**
see PCT Gazette No. 07/2001 of 15 February 2001, Section II

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

CORRECTED VERSION

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
20 January 2000 (20.01.2000)

PCT

(10) International Publication Number
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(51) International Patent Classification[6]: G06F 17/30

(21) International Application Number: PCT/US99/15688

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(25) Filing Language: English

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Filed on 13 July 1998 (13.07.1998)

(71) Applicant *(for all designated States except US)*: **GLAXO GROUP LIMITED** [GB/GB]; Glaxo Wellcome House, Berkeley Avenue, Greenford, Middlesex UB6 0NN (GB).

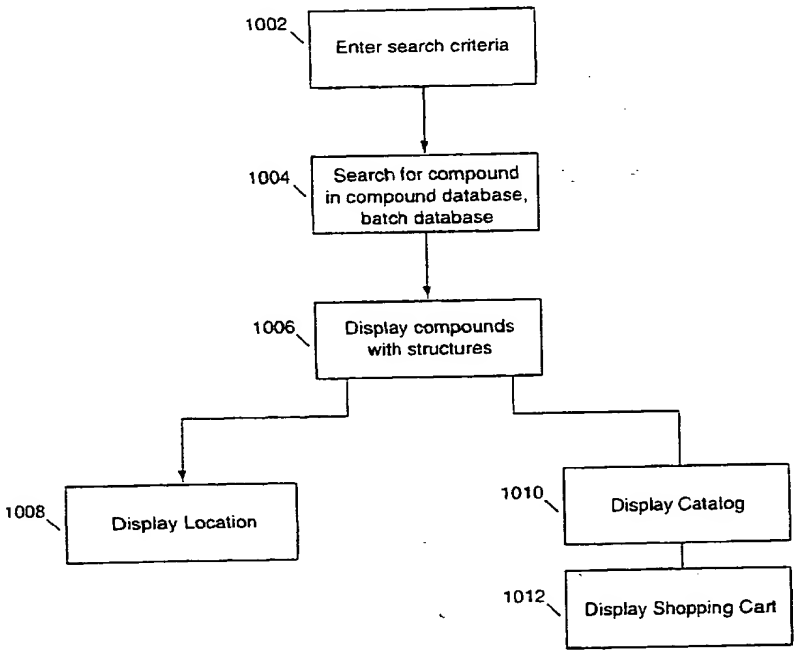
(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: **MUSKAL, Steven, Marc** [US/US]; 2656 Hesselbein Way, San Jose, CA 95148 (US). **EGLI, Paul, Andrew** [US/US]; 39865 Cedar Boulevard #342, Newark, CA 94560 (US). **PENG, Chunyang** [CN/US]; 20650 Park Circle E. #1, Cupertino, CA 95014 (US). **MCGREGOR, Malcolm, James** [GB/US]; 655 S. Fair Oaks Avenue #G302, Sunnyvale, CA 94086 (US).

(74) Agent: **STEVENS, Lauren, L.**; Affymax Research Institute, 4001 Miranda Avenue, Palo Alto, CA 94304 (US).

(81) Designated States *(national)*: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW.

[Continued on next page]

(54) Title: CHEMICAL COMPOUND INFORMATION SYSTEM



(57) Abstract: Systems and methods for managing chemical compound information. Chemical compound tracking and purchasing systems may be provided. A user interface (1002) allows for queries to identify compounds (1004) available internally to the organization and for orders from external sources for compounds that are unavailable internally. Background processing of compound characteristics as stored in a chemical compound database (1004) may be provided (1006).

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CHEMICAL COMPOUND INFORMATION SYSTEM

BACKGROUND OF THE INVENTION

The present invention relates to information systems and more particularly to information systems for chemical compounds.

Operation of the modern chemical laboratory environment requires the management of large numbers of chemical compound containers. These containers may be dispersed over thousands of locations. A researcher or chemist desiring a given chemical compound may be aware of chemical compounds found at his or her location or possibly at nearby locations but is likely to be unaware of chemical compounds available within his or her organization. He or she may conduct a search by physically scanning available contents at many locations or by making successive telephone calls to personnel throughout the organization. It may be more time efficient and thus cheaper to simply order the chemical compound from an external source even if the chemical compound is already available internally.

Even ordering from an external source is complicated by the need to search through numerous supplier catalogs which may not be up to date. After locating the catalog information, completing an order generally requires contacting the supplier by telephone during the supplier's business hours.

A related management problem concerns collecting and maintaining information on the characteristics of chemical compounds. For the purpose of identifying chemical compounds for particular purposes including pharamaceutical purposes, it would be desirable to maintain a chemical compound database that stores for each of many chemical compounds information including: 1) the three dimensional structure of the compound, 2) identification of pharmacaphores of the compound, and 3) a specification of the compound structure that does not include disconnected salt fragments.

SUMMARY OF THE INVENTION

By virtue of the present invention, systems and methods for managing chemical compound information are provided. One embodiment provides a chemical compound tracking and purchasing system. A container database is maintained identifying chemical compound containers available within an organization. A integrated user interface

allows for queries to identify compounds available internally to the organization and for orders from external sources for compounds that are unavailable internally.

Another embodiment of the invention provides background processing of compound characteristics as stored in a chemical compound database. When a chemical compound is registered to a database, its two-dimensional chemical structure is also registered. One or more autonomous processes take this two-dimensional chemical structure as an input to generate additional compound characteristic information to add to the compound database. For example, a first autonomous process may remove salts from stored two-dimensional structures. The removal of salts facilitates searching for useful compounds because salt substructures do not normally affect the ability of one compound to bond with another. A second autonomous process may remove protective groups from the stored structures. These are groups that cleave during synthesis and it is useful to remove them from the compound database to facilitate the evaluation of database products. A third autonomous process may determine a possible three-dimensional structure for each compound, an example of information useful in identifying compounds having desired pharmaceutical characteristics. A fourth autonomous process may identify pharmacaphoric groupings in the stored two-dimensional structures. Knowledge of the pharmacaphores found within each compound greatly facilitates searching for compounds having desired pharmaceutical characteristics.

Another embodiment of the present invention provides for chemical compound registration system having a web-based interface. The web-based interface facilitates entering information about chemical compounds from any location on a network.

A further understanding of the nature and advantages of the inventions herein may be realized by reference to the remaining portions of the specification and the attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 depicts a computer system suitable for implementing one embodiment of the present invention.

Fig. 2 depicts a computer network suitable for implementing one embodiment of the present invention.

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to one embodiment of the present invention.

Fig. 4 is a flowchart describing steps of an overall background process for enriching a chemical compound database in the background according to one embodiment of the present invention.

Fig. 5 is a flowchart describing steps of removing salts from a chemical compound according to one embodiment of the present invention.

Fig. 6 depicts a compound with pharmacaphoric groupings marked and with a salt removed.

Fig. 7 depicts a simplified representation of a laboratory facility.

Fig. 8 depicts a scanner as would be used in one embodiment of the present invention.

Fig. 9 depicts a flowchart describing steps of tracking chemical compound containers according to one embodiment of the present invention.

Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention.

Figs. 11A-11F depict a user interface for locating and purchasing chemical compounds according to one embodiment of the present invention.

Fig. 12 depicts a configuration of pharmacaphoric groupings.

DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides a chemical compound information system. In certain embodiments, the information system includes a chemical compound tracking and purchase system. In certain other embodiments, the chemical compound information system includes a chemical compound registry for registering information about new compounds. This registry may have a web-based interface. Once compounds are registered to a database, background processing may enrich the database with useful information about the compounds such as, e.g., three-dimensional structure, pharmacaphoric groupings, and information about included salts.

Representative Hardware

Fig. 1 shows basic subsystems of a computer system suitable for use with the present invention. In Fig. 1, computer system 10 includes bus 12 which interconnects major subsystems such as central processor 14, system memory 16, input/output (I/O) controller 18, an external device such as a printer 20 via parallel port 22, display screen 24 via display adapter 26, serial port 28, keyboard 30, fixed disk drive 32 and floppy disk drive 33 operative to receive a floppy disk 33A. Many other devices can be connected such as scanning device 34 connected via I/O controller 18, a network interface 35, a mouse 38 connected via serial port 28. Many other devices or subsystems (not shown) may be connected in a similar manner. Also, it is not necessary for all of the devices shown in Fig. 1 to be present to practice the present invention, as discussed below. The devices and subsystems may be interconnected in different ways from that shown in Fig. 1. The operation of a computer system such as that shown in Fig. 1 is readily known in the art and is not discussed in detail in the present application. Source code to implement the present invention may be operably disposed in system memory 16 or stored on storage media such as fixed disk 32 or floppy disk 33A.

Fig. 2 depicts a computer network 200 suitable for implementing the present invention. A central station 202 maintains databases as described herein. Central station 202 is preferably a Unix or Windows NT server such as an ORGIN 2000 server available from Silicon Graphics, Inc. of Mountain View, California. Central station 202 operates databases as described below and preferably provides external access to these databases using standard well-known Internet protocols such as HTTP. Database operation may also be divided among multiple central stations.

A plurality of remote stations 204 may access the databases of central station 202 using HTTP. Database access may be for searching for needed compounds or for registering new compounds. Remote stations 204 operate standard web browsing software such as Netscape Navigator or Microsoft Internet Explorer. Remote stations 204 may be implemented on a wide variety of computer platforms that support such browsing software. Any time of network may interconnect central station 202 including LANs, WANs, the Internet, an intranet, or any combination of these.

Databases Operated

A chemical compound information system according to the present invention may maintain various databases. A chemical compound database may include records corresponding to individual chemical compounds. Each record includes one or more of the representative fields shown in Table 1.

TABLE 1

FIELD	INFORMATION
MOLREGNO	Unique registration number for molecule
MOLNAME	Molecule name
CONV_NAME	Conventional name
IUPAC_NAME	IUPAC name
MOLFORMULA	Molecular formula
MIN_MWT	Minimum molecular weight
MAX_MWT	Maximum molecular weight
REGNO	Organization-wide reg. no.
PUBLISH	Make available to other parts of organization--yes or no?
STORAGE_COND	Storage conditions
SOLUBILITY	Solubility
HANDLEPRECAUT	Handling precautions
STEREO_ISOMER	Whether or not there are stereo isomers
GEOM_ISOMER	Whether or not there are geometric isomers
SAM_COMMENT	Comment
LEGACY_DATE	
PARENT_REGNUM	Registration number of synthesis predecessor

TABLE 1	
FIELD	**INFORMATION**
NUMSPECIFIC_STRUCT	Status of background calculations

Each molecule has a unique registration number, "REGNO." The remaining fields are self-explanatory. "NUMSPECIFIC_STRUCT" indicates the status of background calculations that will be described below. The information in the remaining fields is self-explanatory in the table. The present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

Another database indexed by MOLREGNO may include the two-dimensional structure for each molecule. There are many possibilities for denoting the two-dimensional structure. In one embodiment, a list of atoms and bonds is given to identify the two-dimensional structure.

A batch database may list the chemical compound containers that are available, e.g. within an organization without resort to an external ordering process. Each container within the organization may have a record within the batch database. Table 2 shows representative fields of a record within the batch database. "LOTNUM" and "REGNO" serve as a key to the batch database. It is contemplated that each container be marked with a bar code that has an associated bar code number. Certain fields concern the source of the batch. Other fields identify personnel responsible for the batch. There are also fields to represent whether certain analysis procedures have been conducted and to represent the results. Again, the present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

TABLE 2	
FIELD	**INFORMATION**
REGNO	Reg. number for molecule
LOTNUM	Unique reg. number for batch

TABLE 2

FIELD	INFORMATION
CHEMIST	Responsible chemist
SUPERVISOR	Responsible supervision
CHEM_SOURCE	Identify source
CATALOG NOTEBOOK	Catalog ID or NOTEBOOK#
VENDOR_NAME	Name of vendor
BARCODE	Barcode number
AMOUNT	Amount
AMOUNT_UNIT	Amount units
PURITY_PERCENT	Purity percentage
QC_METHOD	Quality control analysis method used
QC_HPLC	Chromatography applied?
HPLC_FILENAME	Chromatography results file
QC_MS	Mass spectrometry applied?
MS_FILENAME	Mass spectrometry results file
QC_C13NMR	C_{13} NMR applied?
C13NMR_FILENAME	C_{13} NMR results file
QC_HNMR	H NMR applied?
HNMR_FILENAME	H NMR results file
MPLOW	Low melting point
MPHIGH	High melting point
MP_COMMENT	Comment on melting point
BPLOW	Low boiling point
BPHIGH	High boiling point
BP_COMMENT	Boiling point comment
OPTROT	Optical rotation information

TABLE 2	
FIELD	**INFORMATION**
PHYS_STATE	Liquid, solid, or gas
BATCH_COMMENT	Batch comment
HANDLE_PRECAUT	Handling precautions
STOR_COND	Storage conditions
ASSIGNED_OTHER_ REGNO	Other Organization reg. no.
GCMS_FILENAME	Gas chromatograph results
QC_GCMS	Gas chromatography applied?
LOCATION	Room
PLACEMENT	Position within room

The databases are preferably maintained as Oracle relational databases at central station 202. External access to the databases is provided by the Enterprise Server program available from Netscape.

Registry System

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to the present invention. This registration system allows users to register proprietary and commercially available chemical compounds into the chemical compound database. Fig. 3A depicts a top portion 300 of a registration form. Fig. 3B depicts a bottom portion 302 of this registration form. This registration form and the other displays of the interface are preferably stored at central station 202. The web browser at one of remote stations 204 requests the registration form using an HTTP request message. The HTTP request is directed to an address of central station 202 and includes an address (any identification information) of the registration form at central station 202. In response to the HTTP request, central station 202 forwards the registration form to remote station 204 for display. Central Station 202 may dynamically generate the registration form. The registration form is communicated to remote station

204 as an HTML document. This process for presenting a web-based interface may be used for all the user interfaces discussed herein.

The registration form shows locations to enter the fields of Table 2. By selecting a structure area 304, the user invokes a chemical structure drawing tool to designate a two-dimensional chemical structure. By selecting a button 306, the user may reset the contents of the form. To proceed to the next screen of the registration interface, the user selects a registration preview button 308. Once the user selects registration preview button 308, the chemical compound information system compares the entered two-dimensional structure of the compound to the structures of the compounds already stored in the compound database to determine if the new compound has already been registered before.

Fig. 3C depicts an upper portion 310 of a registration preview form. Fig. 3D depicts a lower portion 312 of this registration preview form. The registration preview form includes a message 314 indicating whether or not the molecule is new to the compound database. Upon user selection of a commit button 316, the entered information will be added to the batch database. If the molecule is new, a new record is also added to the compound database.

Also, after the user selects commit button 316, the chemical compound information system displays a registration report form. Fig. 3E depicts an upper portion 318 of this registration report form. Fig. 3F depicts a lower portion 320 of this registration report form. The registration report form confirms the information that has been registered, gives a registration number 322 corresponding to "REGNO", and a time and date 324 of registration.

Operating this registry system over the web is highly beneficial. The user interface is easy to use and can be accessed from any location accessible via the network. In some embodiments, the registry system operates over the Internet permitting registration to occur anywhere in the world.

Background Autonomous Enrichment

Fig. 4 is a top level flowchart describing steps of a background process for enriching the compound database according to one embodiment of the present invention. The background process may operate autonomously without invocation by any user. The

background process sequentially goes through the records of the compound database (step 402) and checks if: (i) the 2 dimensional (2D) structure has been processed (step 404), and (ii) a 3 dimensional (3D) structure, corresponding to the 2D structure, has been added (step 410). If either of these have not been performed the following processes are put into operation depending on which process or processes need to be done.

Preparing the 2D structure preferably involves the application of 2 processes: StripSalt (step 406) and StipProt (step 408) , described below.

StripSalt:

Compounds obtained from commercial suppliers often contain salts which appear in the database as part of the molecule structure; this aids the laboratory chemist but interferes with structure calculations. The program stripsalt identifies disconnected fragments based on the bond connectivity data, and outputs only the largest connected fragment, which is assumed to be the molecule of interest. The technique is given in Fig. 5. It assumes that the structure record contains a list of covalent bonds, each of which connects 2 atoms.

Fig. 5 is a flowchart describing steps of removing disconnected fragments based on bond connectivity data according to one embodiment of the present invention. At step 502, the procedure starts at the first bond. At step 504, the procedure checks whether the both atoms in the bond are without a fragment label. If yes, the procedure assigns a new fragment label to both atom at step 506. If no, the procedure goes to step 508 where it checks whether only one atom in the bond has a fragment label. If yes, the procedure assigns the fragment label of the labeled atom to the unlabeled atom at step 510. If no, the procedure goes to step 512 where it checks if the fragment labels of both atoms are different. If yes, the procedure goes to step 514 where it goes through every atom in the molecule and for those atoms labeled with the same fragment as the second atom in the current bond, it changes the fragment label to match the first atom in the current bond.

Upon a finding of no difference at step 512, and after any one of steps 506, 510, and 514, the procedure checks at step 516 whether the current bond is the last bond. If the current bond is not the last bond, the procedure goes to the next bond at step 518. If the current bond is the next bond, the procedure goes to step 520. At step 520, the

procedure counts the number of atoms in each fragment and outputs only the atoms and bonds in the largest fragment. The smaller fragment is the salt that is removed.

StripProt:

Frequently chemical reagents contain protecting groups which are cleaved during synthesis. It may be preferable to remove them from the database structure. This is important if the structure is used as an input to a database reaction scheme, ensuring that the resulting product structure resembles the actual chemical product. StripProt reads a set of protecting groups as chemical structures from an input file and does a substructure search on the database structure. The input file also contains information about which atoms in the substructure are to be removed when a substructure match is found. The file is an ASCII file which contains a definition of its own format and as such can be modified by the user. The substructure search is an atom by atom mapping algorithm as described in Gluck, D.J. "A Chemical Structure Storage and Search System Developed at Du Pont", J. Chem. Doc. 1965, 5, 43-51, the contents of which are herein incorporated by reference.

Generation and processing of the 3D structure involves 2 main steps: (i) calculation of 3D coordinates (step 414), and (ii) addition of pharmacophoric labels (step 412). The 3D structure is then added to the database. The 3D coordinates are calculated using the Corina program from Oxford Molecular. The pharmacophoric labels are calculated by the program AddPharm, below.

Addpharm:

Identifies pharmacaphoric groups which are relevant to drug design. They are defined as substructures in an input file which are chosen using heuristics about which substructures contain the pharmacophoric groups. For example a carboxylate has a negative charge, aliphatic amine has a positive charge, hydroxyl is both a hydrogen bond donor and acceptor, and so on. The file is an ASCII file which contains a definition of its own format and can be modified by the user. The database structures are searched using the same substructure search algorithm as in StripProt. When there is a substructure hit, the file contains information about which atoms to label with which pharmacophoric type, and these are added as records in the database. The pharmacophoric groups include the following types: A: hydrogen bond acceptor, D:

hydrogen bond donor, H: hydrophobic, N: negatively charged, P: positively charged and R: aromatic. These represent the kinds of interactions observed when a small molecule ligand binds to a protein receptor. A pharmacophore is then a set of such points in a spatial arrangement which represents the interactions made with a particular protein receptor. Therefore the other procedure needed for a full pharmacophore search is a conformation generator; this may be a feature of the database or may be done by an external program.

Fig. 6 depicts a representative compound, sumatriptan succinate. The added pharmacophoric labels are shown. A succinate salt 704 can be seen to be a disconnected fragment and is therefore removed.

Compound Tracking and Acquisition

Fig. 7 is a simplified representation of a laboratory environment where systems and methods according to the present invention may be deployed. A laboratory facility 700 includes a plurality of rooms 702. Each room 702 is preferably equipped with at least one wall-mounted scanner 704 for scanning in chemical compounds. Although, Fig. 7 depicts a single scanner 704 in each room 702, there may be multiple scanners in each room. Any type of data entry device may substitute for the scanners 704. Shelves 706 store containers of chemical compounds. Each depicted room 702 is assumed to be used for experiments or chemical processing. A chemical stock room is not needed. Laboratory facility 700 is merely representative of environments where a compound tracking and acquisition system may be deployed. A compound tracking or acquisition system may be implemented in any physical environment according to the invention.

Fig. 8 depicts details of scanner 704. Scanner 704 includes a scanning wand 802 for reading bar codes from chemical compound containers. Scanning wand 802 is preferably an Intermec 1545 non-contact bar code scanner available from Intermec, Inc. of Everett, Washington. A fixed portion 804 of scanner 704 includes a display 806 for presenting user prompts, a keyboard 808, and an RF unit 810 including an antenna 812. Except for RF unit 810 and antenna 812, fixed portion 804 may be a 9560 transaction manager available from Intermec.

In one scenario, when a container arrives in a facility receiving department, a preprinted barcode label is affixed to the outer packaging. A single box including many containers may have several labels. The containers are then initially registered in the database on central station 202. The containers are delivered to individual rooms 702 where the bar codes are scanned in. Whenever a container moves it is rescanned.

Fig. 9 is a flowchart describing steps of registering a new location for a chemical compound container according to one embodiment of the present invention. At step 902, a user waves wand 802 over a bar code on a chemical container. Once the bar code has been read, RF unit 810 transmits the new location information to central station 702 at step 906. RF unit 810 preferably operates around 800 MHz. Central station 202 is similarly equipped with RF receiver equipment (not shown). At step 908, central station 202 modifies the container location information in its database. Preferably, the DataConnect program available from Connectware, Inc. of Santa Clara, California interfaces between the scanner system and the databases described above.

Optionally, a user may register consumption of compound even without change of location by scanning the bar code and making appropriate entries on keyboard 808. The user may also similarly register complete depletion of the bottle contents and automatically reorder fresh stock.

Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention. Fig. 10 will be described with reference to Figs. 11A-11F which illustrate a user interface for acquiring a chemical compound. An advantage provided by virtue of the present invention is the ability to use an interface both for searching for a compound internally, and for acquiring the compound from an external source. The user interface is assumed to be active at one of remote stations 204, although it would of course be also possible to operate it at central station 202. In a preferred embodiment, the interface is web-based.

At step 1002, the user enters search criteria giving characteristics of the desired compound. Fig. 11A depicts the user interface for this step. The user may enter a chemical name or a chemical formula. Other textual or numerical criteria include the amount of chemical compound desired, the registration number, the catalog number or the location.

The user may also enter the structure in a structure area 1102 to find a compound having the same or similar structure to the entered structure. The user may also use structure area 1102 specify a substructure that would be found within the desired compound. The user may also specify a configuration of pharmacaphoric groupings that can be presented by the compound as shown in Fig. 12. Fig. 12 depicts that an acceptor 1202, donor 1204, and aromatic 1206 are presented. To meet the bonding criterion determined by the depicted configuration, a compound must be able to present these pharmacaphoric groupings at the spacings indicated in Fig. 12. A pull-down menu 1104 is used to select among these various types of structural criteria.

At step 1004, central station 202 searches for compounds having the desired characteristics in the compound database and the batch database. At step 1006, remote station 204 displays the structures of compounds having characteristics matching the search criteria. A representative display for this step is depicted in Fig. 11B. For each compound the display shows a structure 1106, a registration number 1108 for the compound. When the compound is available internally, one or more location codes are also shown. When the compound is available externally, the number of suppliers 1110 is shown. Fig. 11C depicts an alternative view of the search results where more information is depicted including a molecule name 1112, a molecular formula 1114, and a molecular weight 1116.

At step 1008, by clicking on any displayed location code, the user can call up a display of a site map which the user may refer to find the physical location of the desired compound. Fig. 11D shows such a site map display 1118. In an alternative embodiment, the display may show a special icon at the location of the compound, or may show directions to the location of the compound from the user's location.

At step 1010, by clicking on the number of suppliers 1110, the user may call up a catalog display 1120 as shown in Fig. 11E. Catalog display 1120 lists vendors, and for each vendor, catalog entries for compounds satisfying the search criteria. For each catalog entry, the display may further include a purity percentage, an indicator of quantity per batch, and a price. The user may specify a desired quantity in one of quantity boxes 1122 and specify a particular catalog entry for order by clicking in one of "add to cart" boxes 1124. When the user is ready to add all of the desired catalog entries to a "virtual shopping cart," the user selects an add to cart button 1126.

Fig. 11F depicts a virtual shopping cart 1128 that lists desired compounds and their previously selected sources. Virtual shopping cart 1128 is displayed at step 1012. A current total price 1130 is given. The user can place an order for the selected items by selecting a place order button 1132. The user can also name the cart for future reference by selecting a name this cart button 1134, clear the cart by selecting a clear cart button 1136, or select a new cart by selecting a new cart button 1138. In one embodiment, when the user selects the cart, the orders are sent to a purchasing department. In another embodiment, when the user selects the cart, the orders are sent directly to the suppliers over the Internet. Payment information may be included with the electronic orders.

The result is a virtual inventory system that allows users to obtain desired compounds quickly and efficiently from both internal and external sources. Benefits include lower cost acquisition since compounds are only requested if they are not available internally, savings in search manpower, and better tracking of costs.

In the foregoing specification, the invention has been described with reference to specific exemplary embodiments thereof. It will, however, be evident that various modifications and changes may be made thereunto without departing from the broader spirit and scope of the invention as set forth in the appended claims and their full scope of equivalents. For example, in any depicted flowcharts, steps may be deleted, substituted, or reordered within the scope of the present invention. Any user interface depicted as being web-based may also be implemented locally, or using any network protocol. For web-based implementations, links may be provided among any combination of the user interface displays to permit free navigation.

WHAT IS CLAIMED IS:

1. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously invoking a three-dimensional structure evaluation routine to determine a three-dimensional structure of said compound based on said two-dimensional chemical structure as a part of said background database management process.

2. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove salts from said two-dimensional chemical structure.

3. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove protective groups from said two-dimensional chemical structure.

4. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database and 3D structures;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said 3D-dimensional chemical structure to identify pharmacaphores in said 3D-dimensional chemical structure.

5. A computer-implemented method for facilitating acquisition of chemical compounds comprising the steps of:

operating an available compound database identifying chemical compounds available within an organization;

accepting user input identifying a desired chemical compound;

searching for said desired chemical compound within said available compound database; and

presenting information concerning availability of said desired chemical compound within said organization and availability from at least one external source.

6. The system of claim 5 wherein said database comprises a plurality of records, each record associated with a particular chemical compound container and indicating a last known location of said chemical compound container.

7. A computer-implemented method for procuring a desired chemical compound comprising:

a) accepting user input indicating a desired chemical compound;

b) searching for one or more container holding said desired chemical compound in a first database, said first database listing available chemical compound containers and their locations; and

c) if no container holding said desired chemical is found in said b) step, searching a second database for said desired chemical compound, said second database storing ordering information for a plurality of chemical compounds.

8. The method of claim 7 wherein said user input comprises a name of said desired chemical compound.

9. The method of claim 7 wherein said user input comprises a chemical structure of said desired chemical compound.

10. The method of claim 7 wherein said user input comprises a chemical substructure found within said desired chemical compound.

11. The method of claim 7 wherein said user input comprises a chemical structure similar to a chemical structure of said desired chemical compound.

12. The method of claim 7 further comprising:

if any container of said desired chemical compound is found in said first database, displaying a location of said container.

13. The method of claim 7 further comprising:

if said desired chemical compound is found in said second database, displaying ordering information for said desired compound.

14. The method of claim 13 further comprising:

accepting user input ordering said desired compound; and

relaying said user input ordering said desired compound to a chemical compound source via a network.

15. A computer-implemented method for registering a chemical compound to a remote database comprising:

accepting user input at a local client specifying an address of a compound input form at a remote server;

in response to said user input, sending a request for said compound input form to said remote server;

in response to said request, transferring data representing said compound input form from said remote server to said local client;

based on said data, displaying said compound input form at said local client, said compound input form including fields for holding compound characteristics;

accepting user input at said local client specifying contents of one or more of said field;

forwarding said contents from said local client to said remote server; and

adding said contents to a compound database accessible by said remote server.

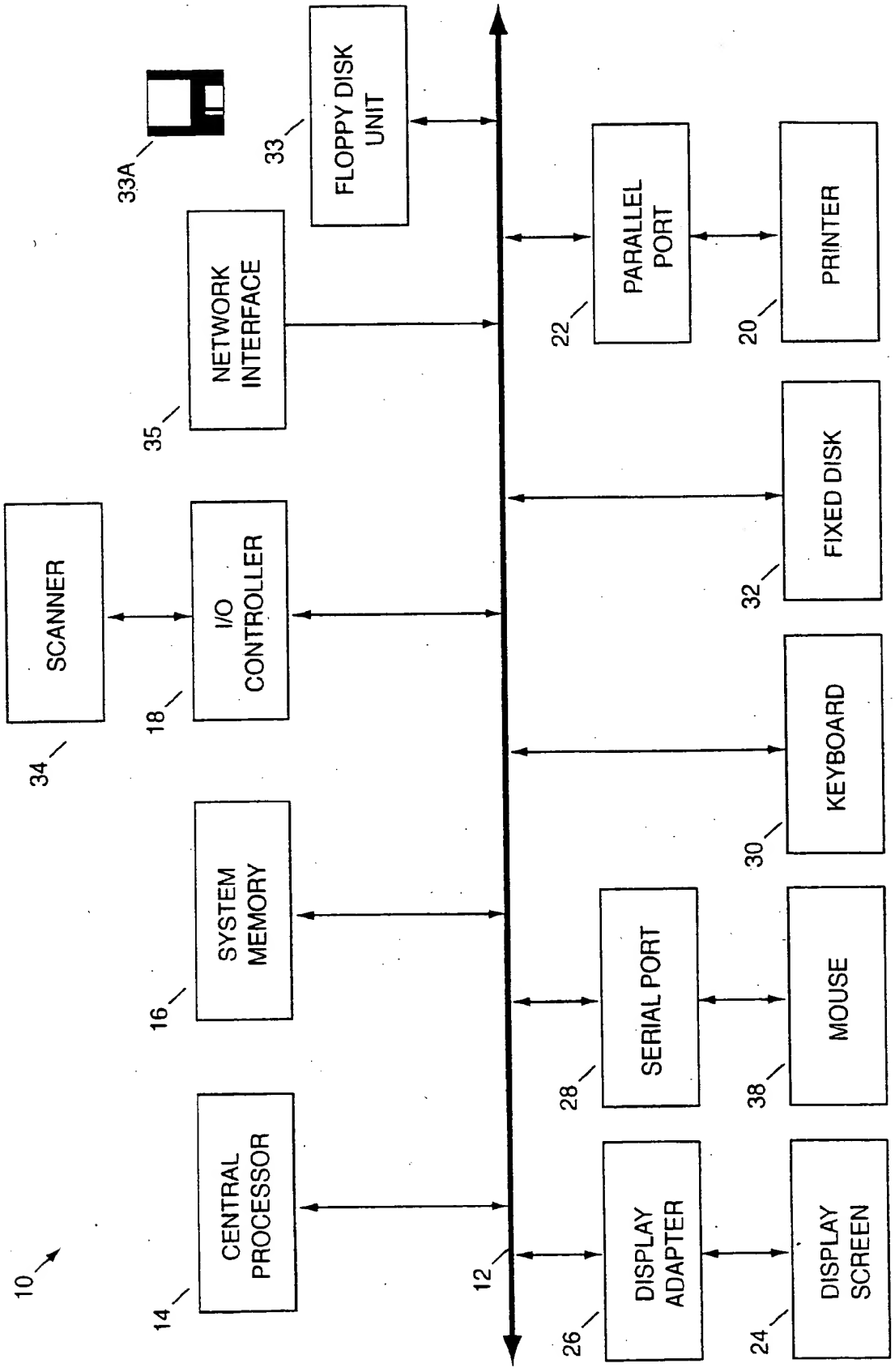


FIG. 1

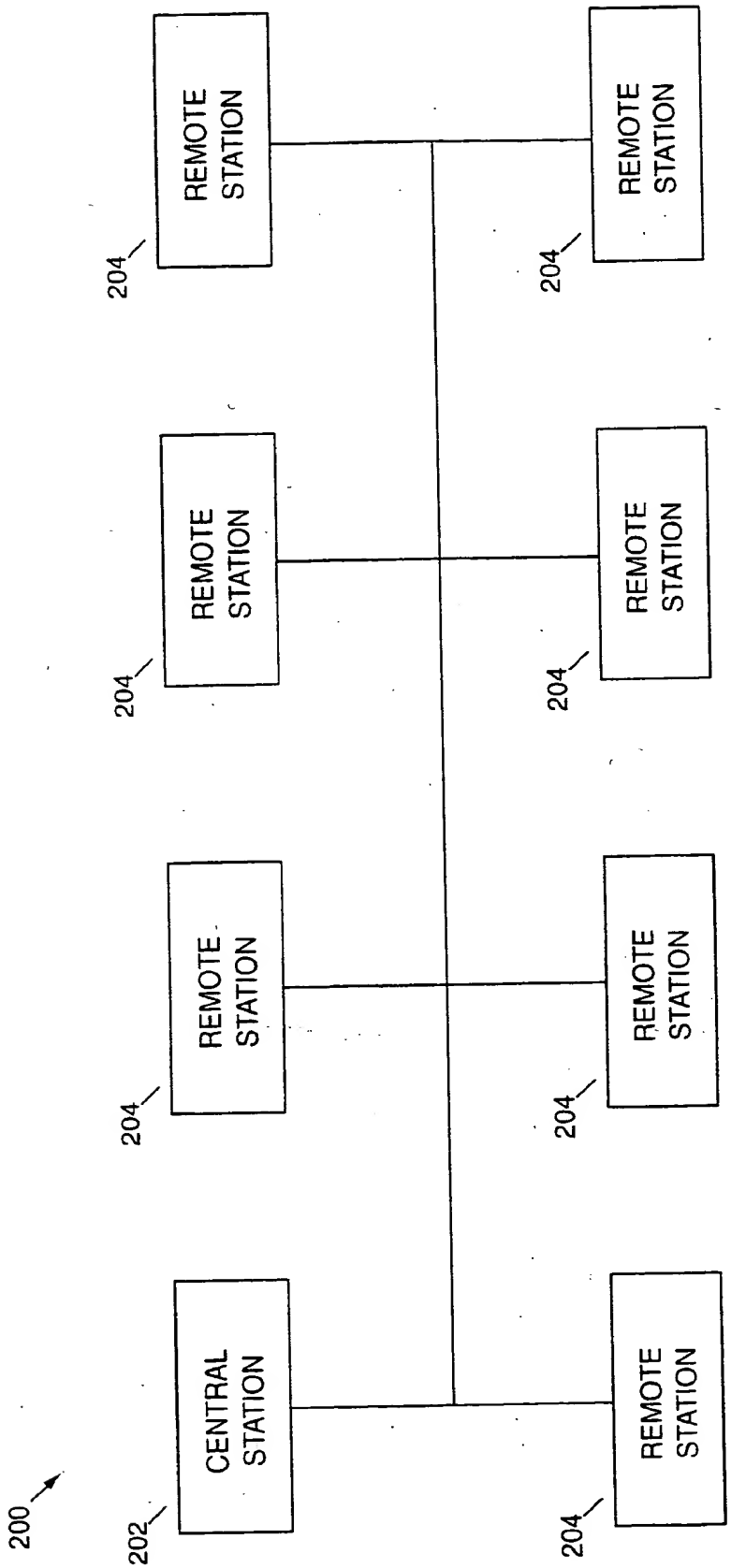


FIG. 2

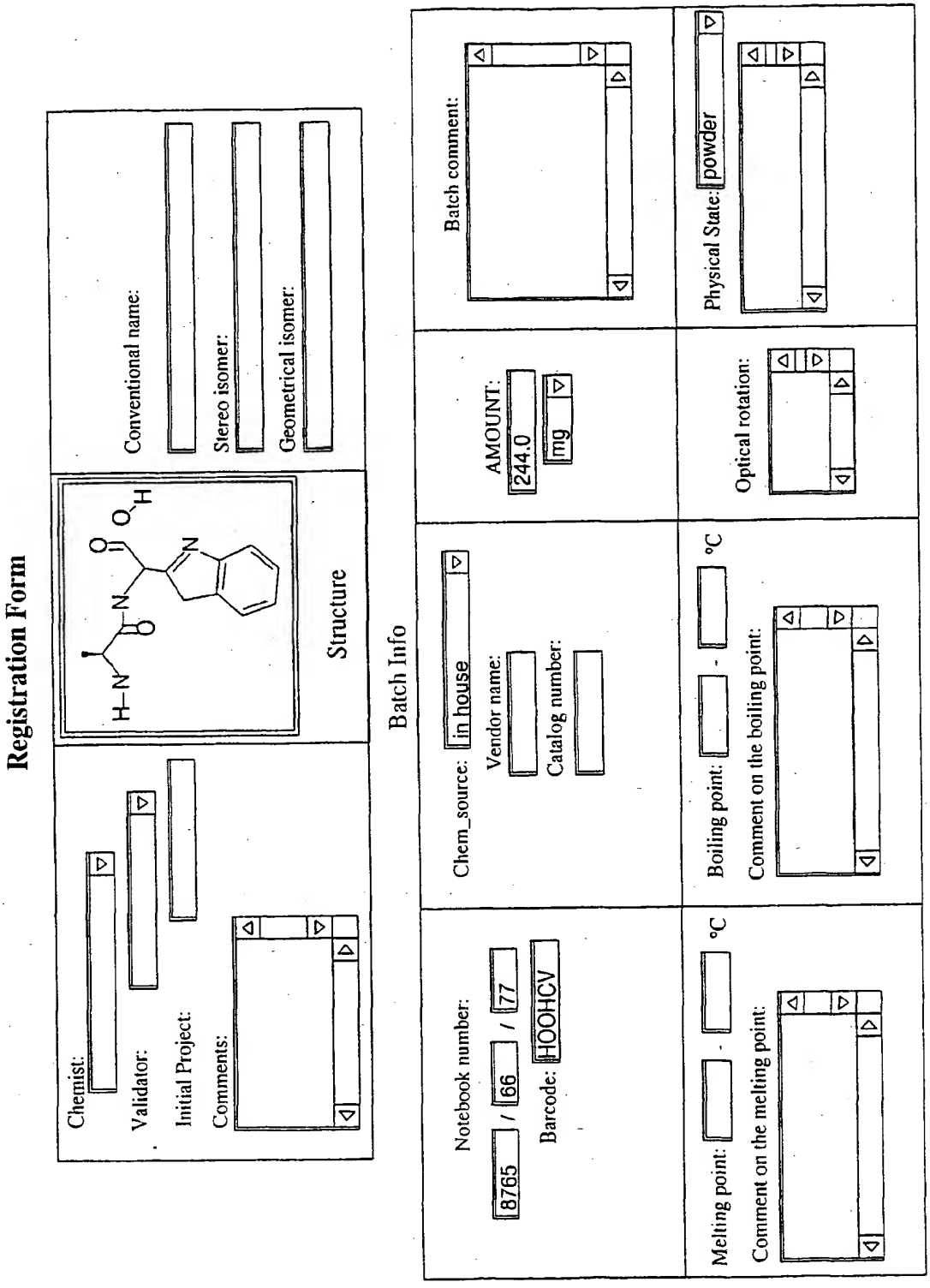


FIG. 3A

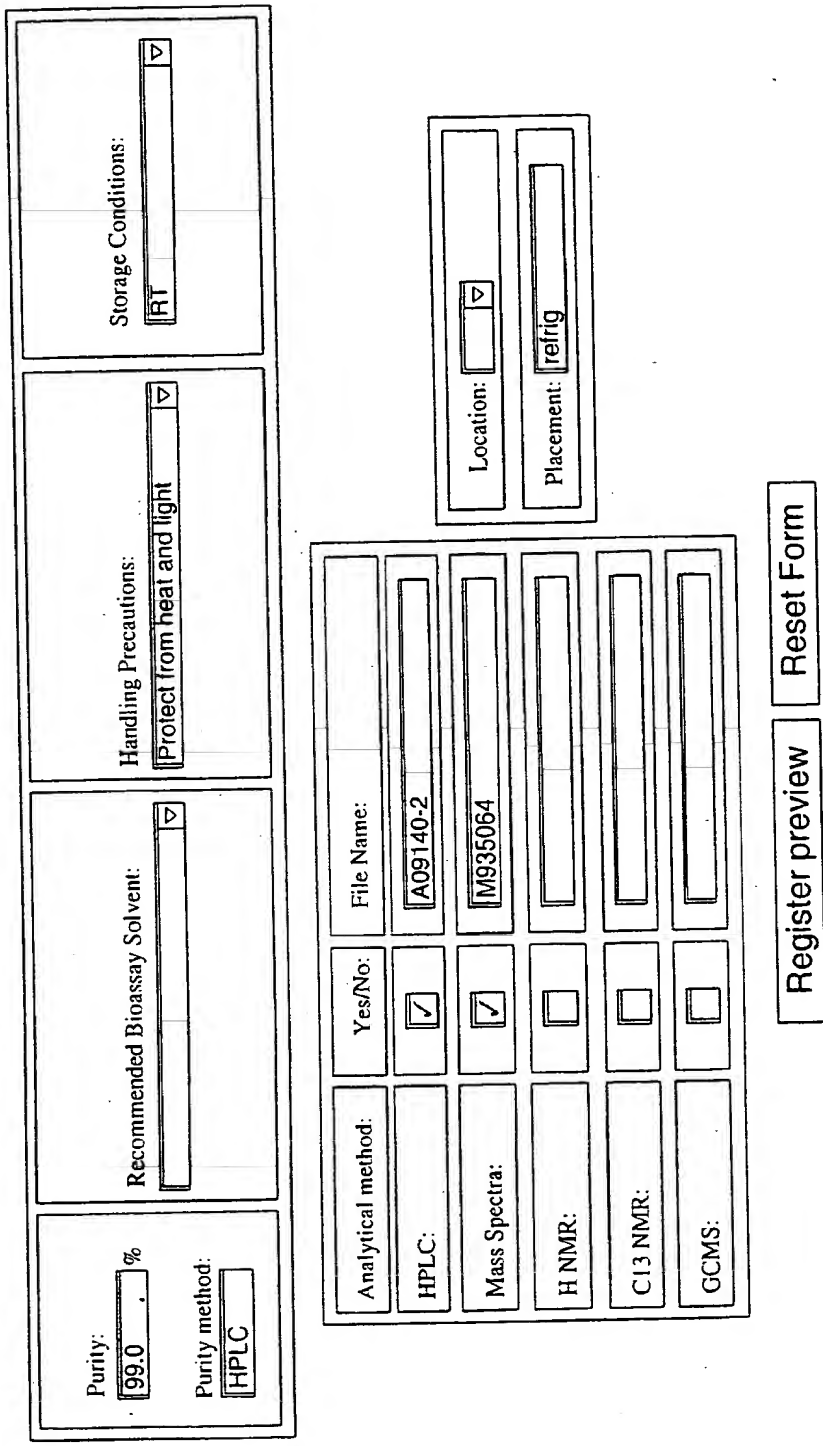


FIG. 3B

Registration Preview Form

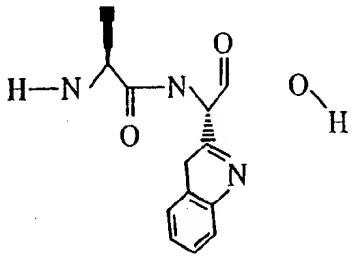
The molecule is new to the database.

The structure and batchinfo will be registered if you commit.

Commit

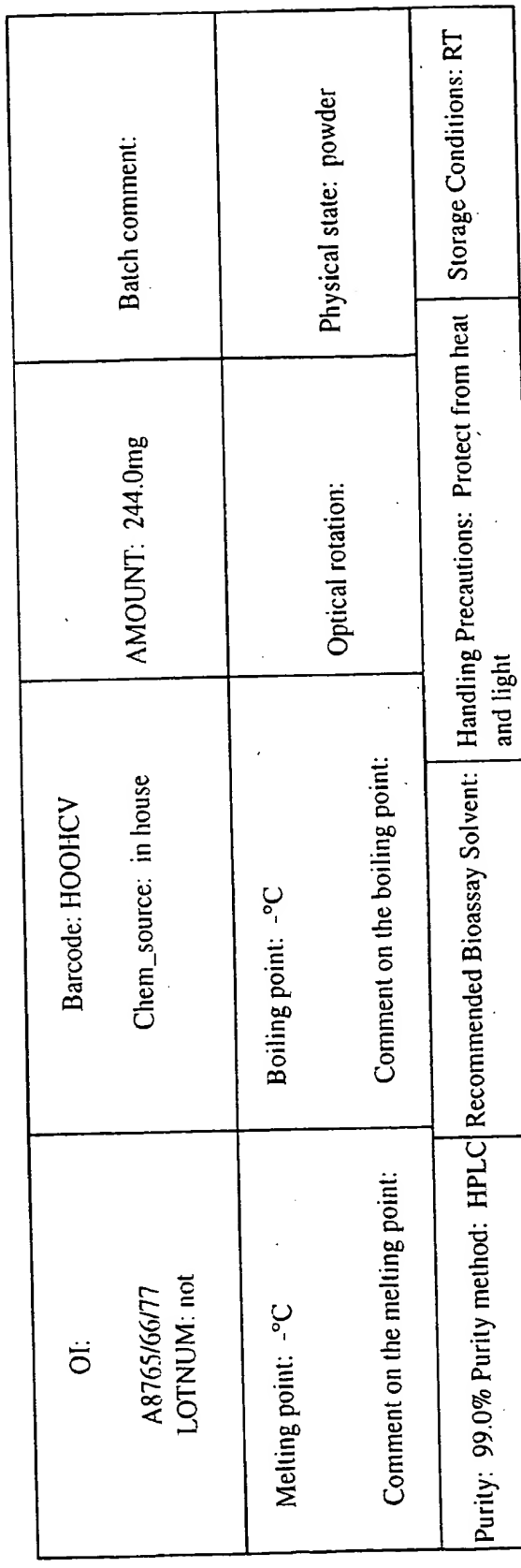
314

ChemBank sample info:

Mol regno number is: no info Chemist: Validator: Initial Project: Molecular Weight: Molecular Formula:	 Structure	Conventional name: Stereo isomer: Geometrical isomer: Comments:

310

FIG. 3C



Analytical method:	Yes/No:	File Name:
HPLC:	Y	A09140-2
Mass Spectra	Y	M935064
H NMR:	N	
C13 NMR:	N	
GCMS:	N	

Location:
Placement: refrig

312

FIG. 3D

ChemBank Registration Report Form

324

month ☐ date ☐ year ☐ time: ☐

322

Your assigned compound registration number is: CB10093

ChemBank sample info:

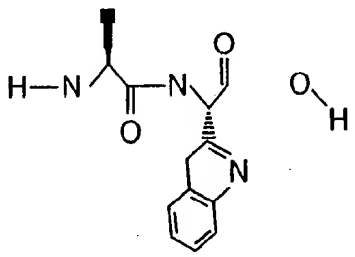
AF number is: CB10093 Chemist: Initial Project: null Validator: Molecular Weight: Molecular Formula:	 Structure	Conventional name: Stereo isomer: Geometrical isomer: Comments:

FIG. 3E

OI: A8765/66/77 LOTNUM: 1	Barcode: HOOHCV Chem_source: in house	AMOUNT: 244mg	Batch comment: null
Melting point: 0-0 °C Comment on the melting point:	Boiling point: 0-0 °C Comment on the boiling point:	Optical rotation:	Physical state: powder
Purity: 99% Purity method: HPLC	Recommended Bioassay Solvent: null	Handling Precautions: Protect from heat and light	Storage Conditions: RT

Analytical method:	Yes/No:	File Name:
HPLC:	Y	A09140-2
Mass Spectra	Y	M935064
H NMR:	N	
C13 NMR:	N	
GCMS:	N	

Location: null
Placement: refrig

320

FIG. 3F

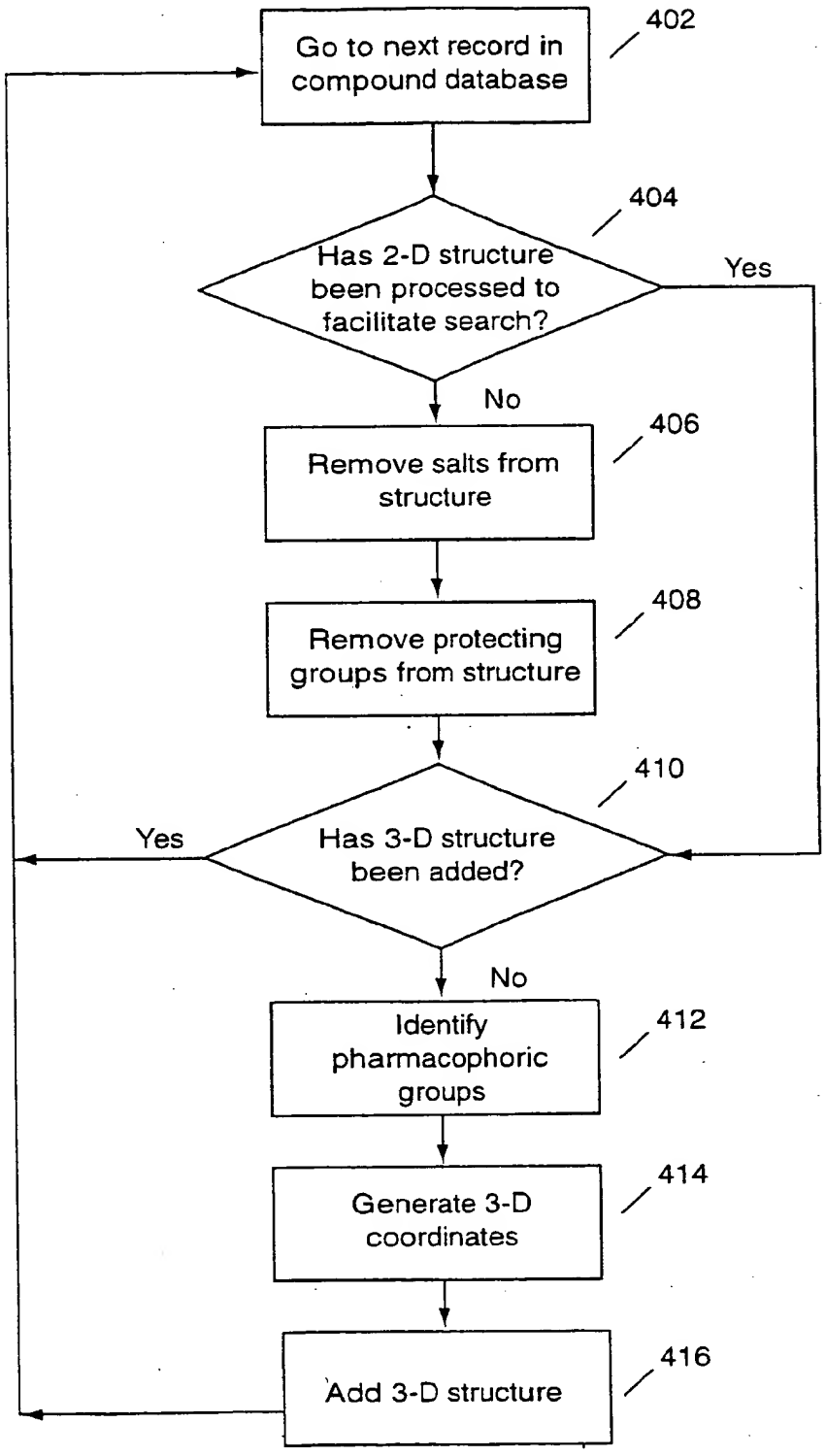


FIG. 4

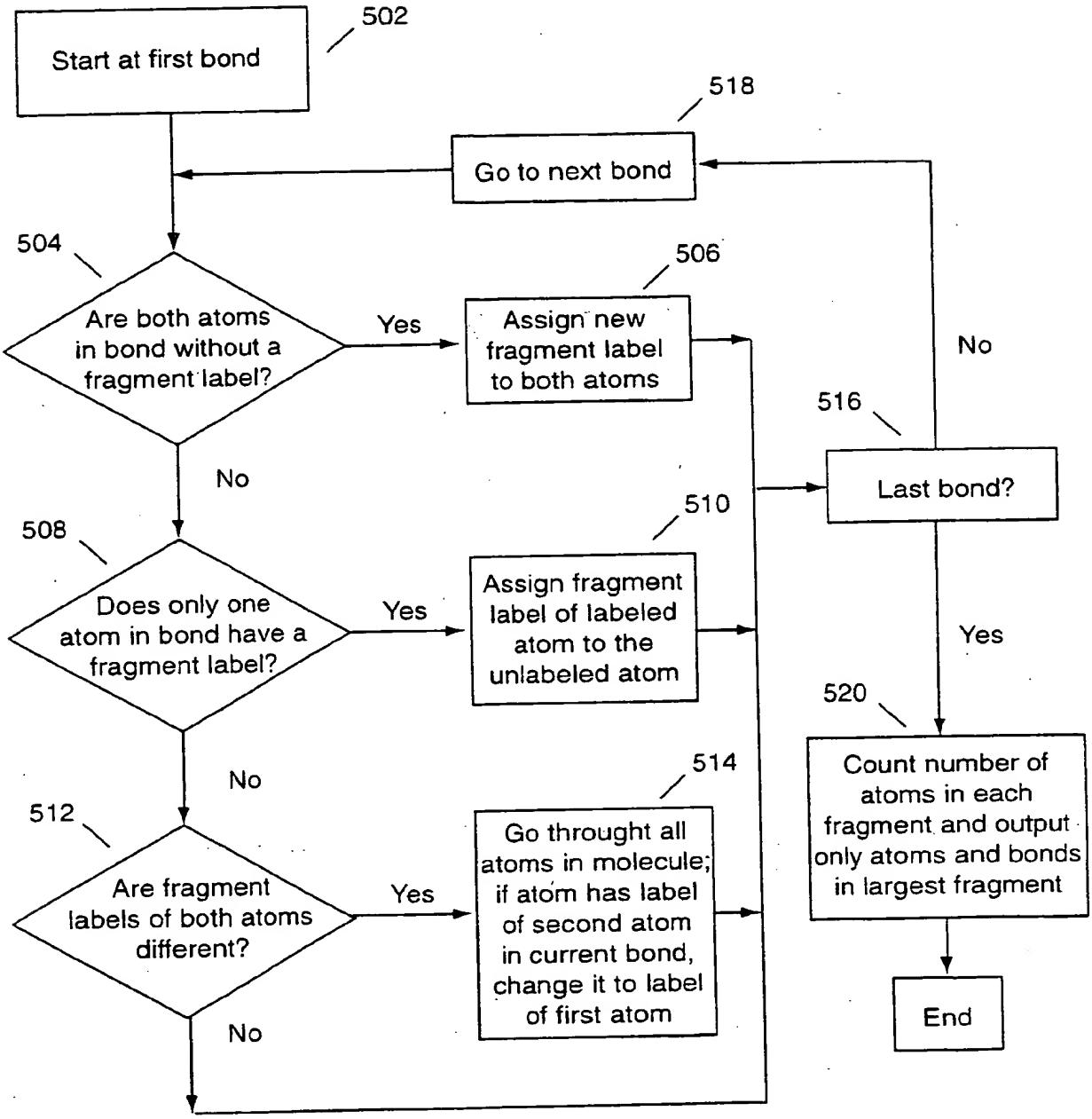


FIG. 5

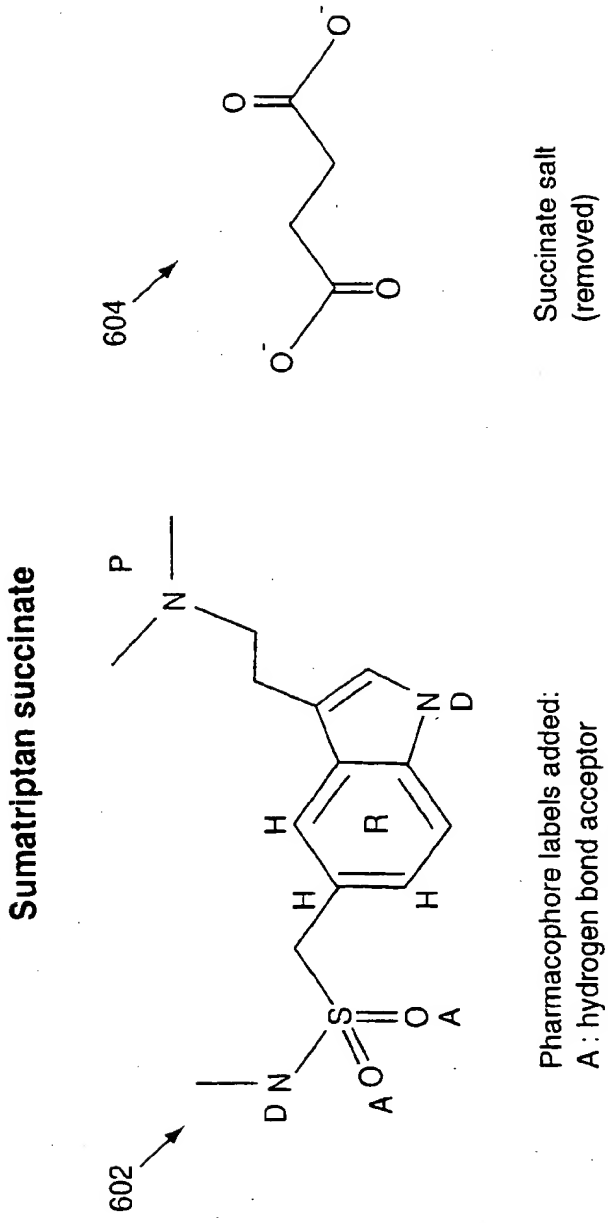


FIG. 6

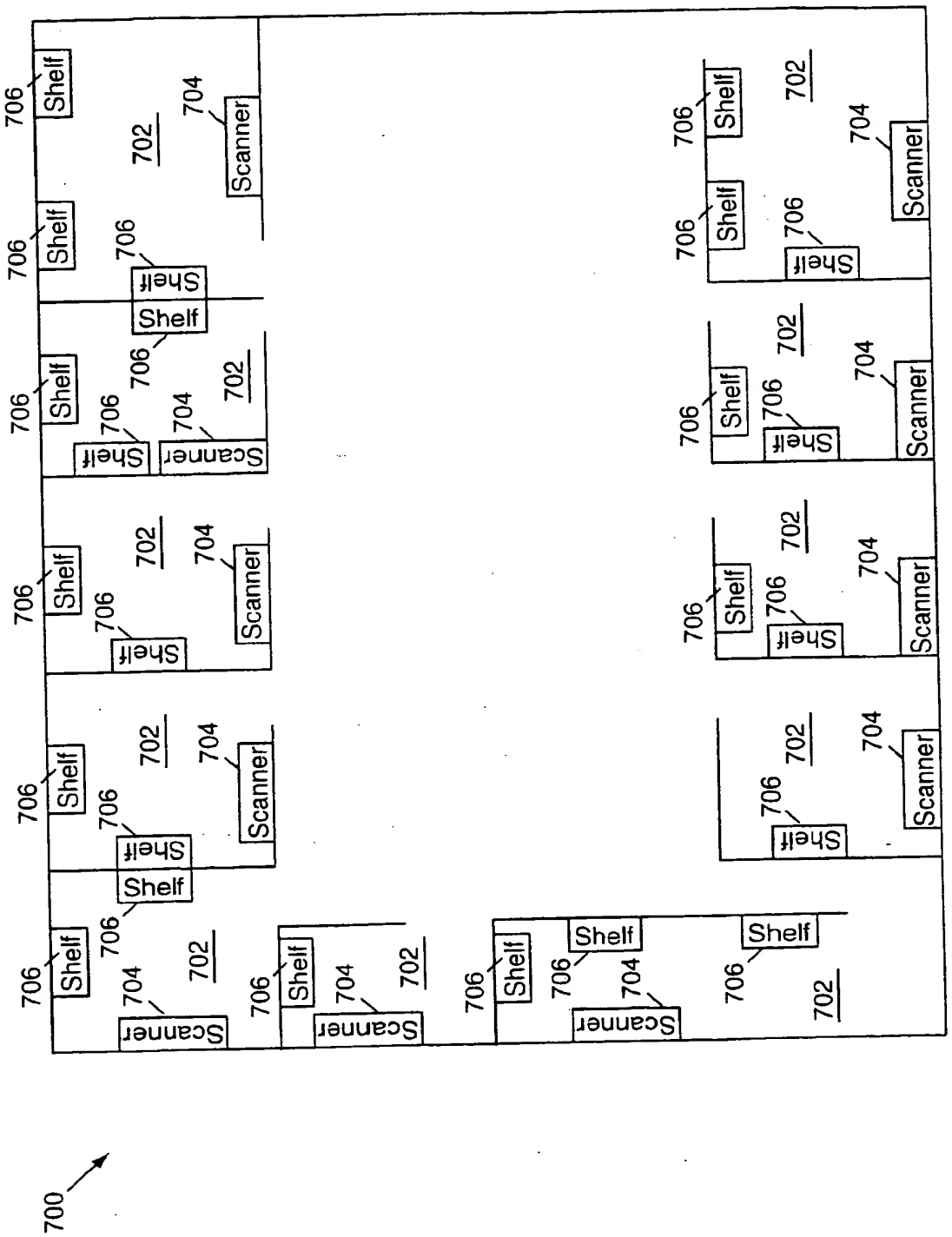


FIG. 7

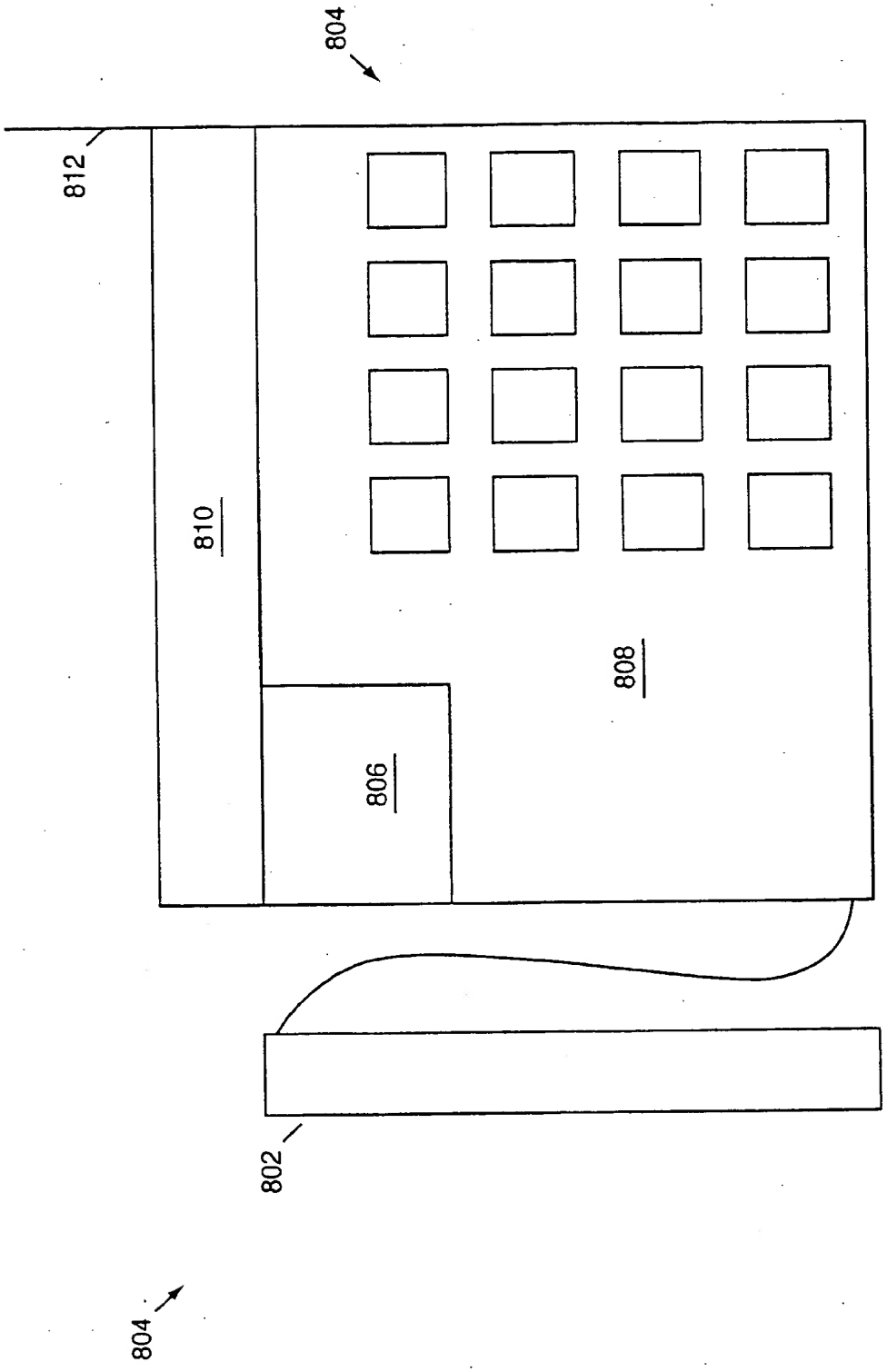


FIG. 8

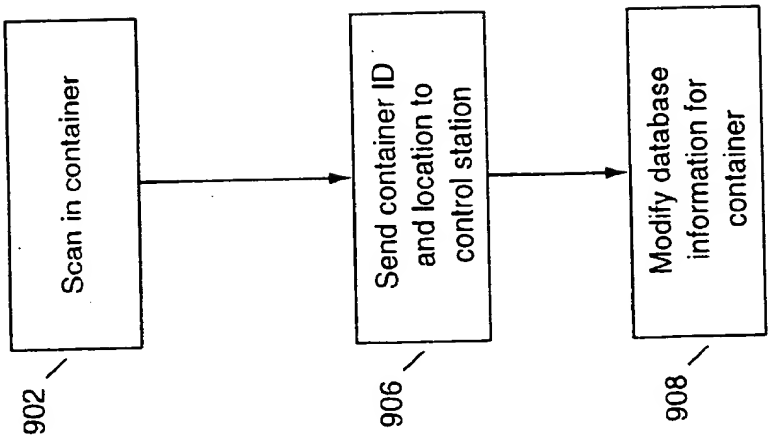


FIG. 9

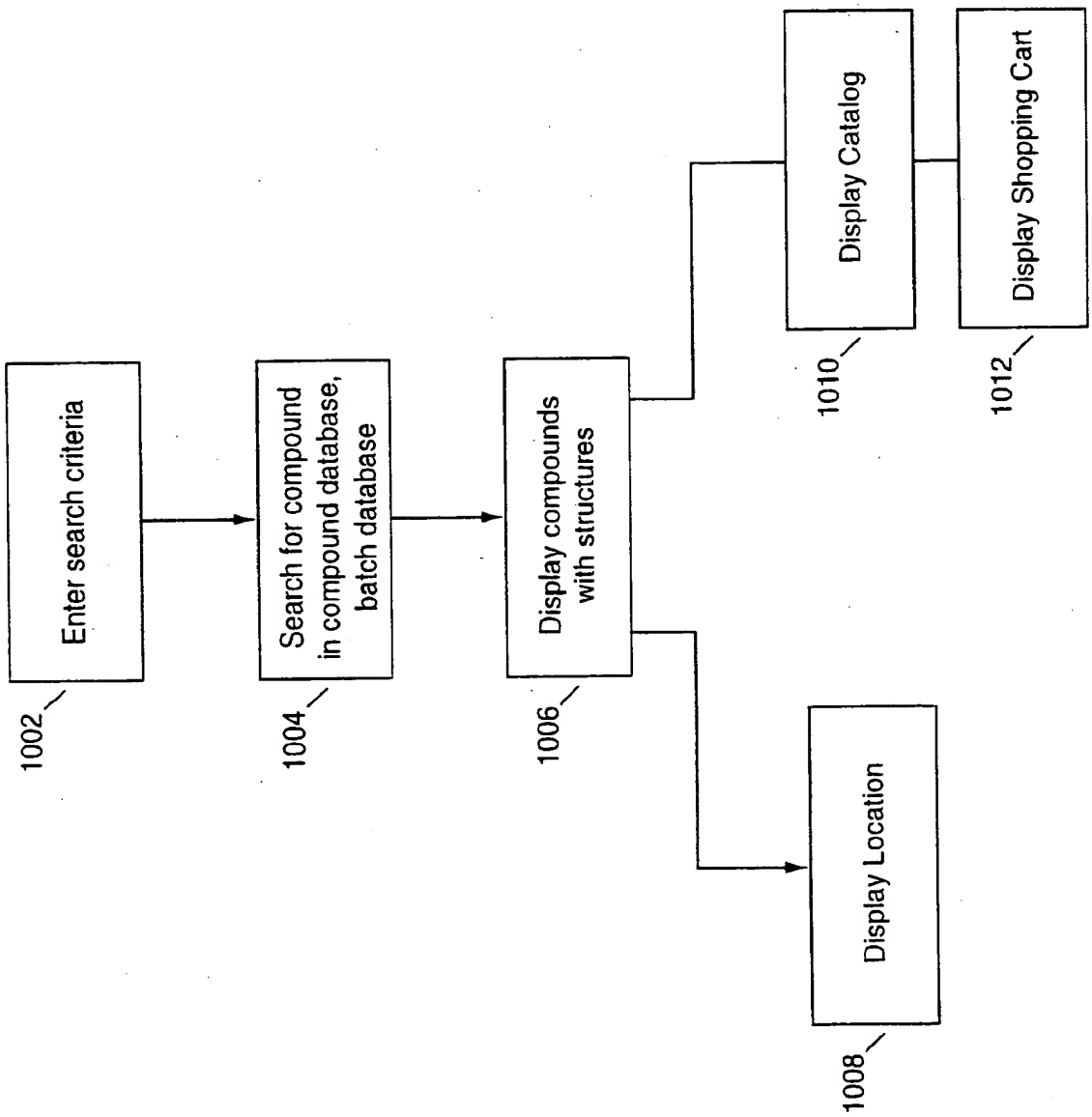


FIG. 10

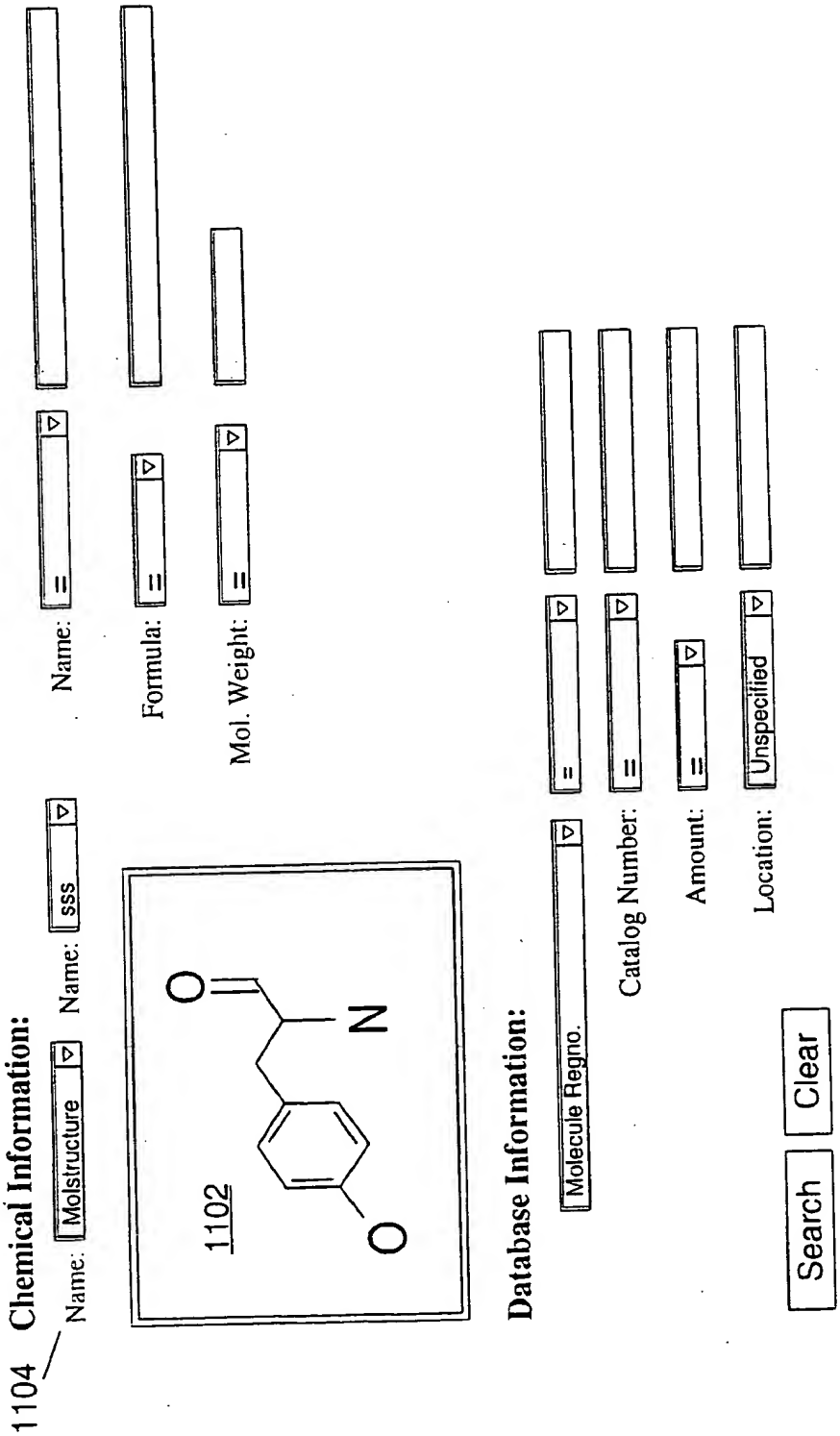
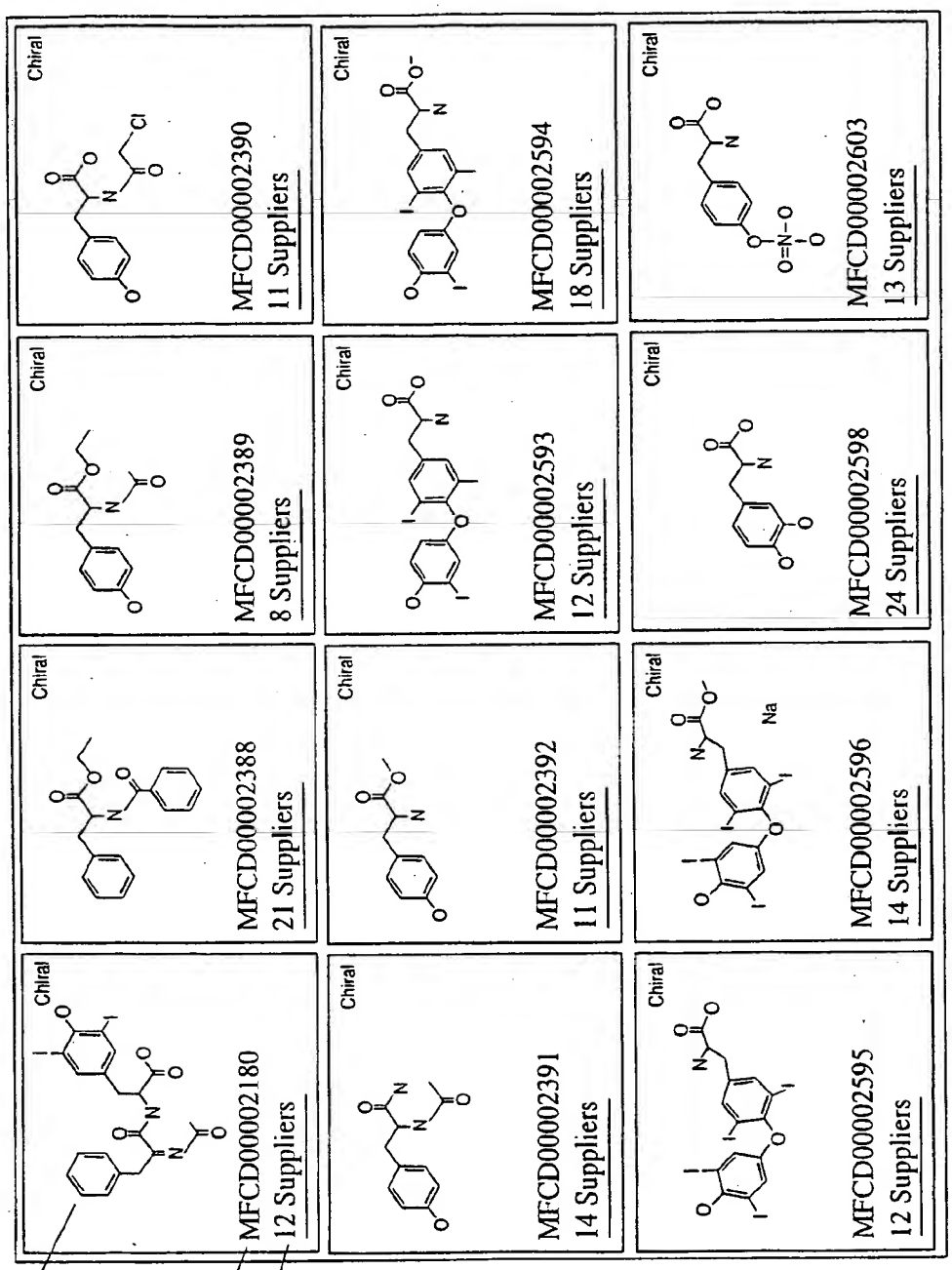


FIG. 11A


Search Results 1 - 20 of 2044
Chiral
MFCD00002180
12 Suppliers
Chiral
MFCD00002388
21 Suppliers
Chiral
MFCD00002389
8 Suppliers
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11 Suppliers
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1106
1108
1110

FIG. 11B

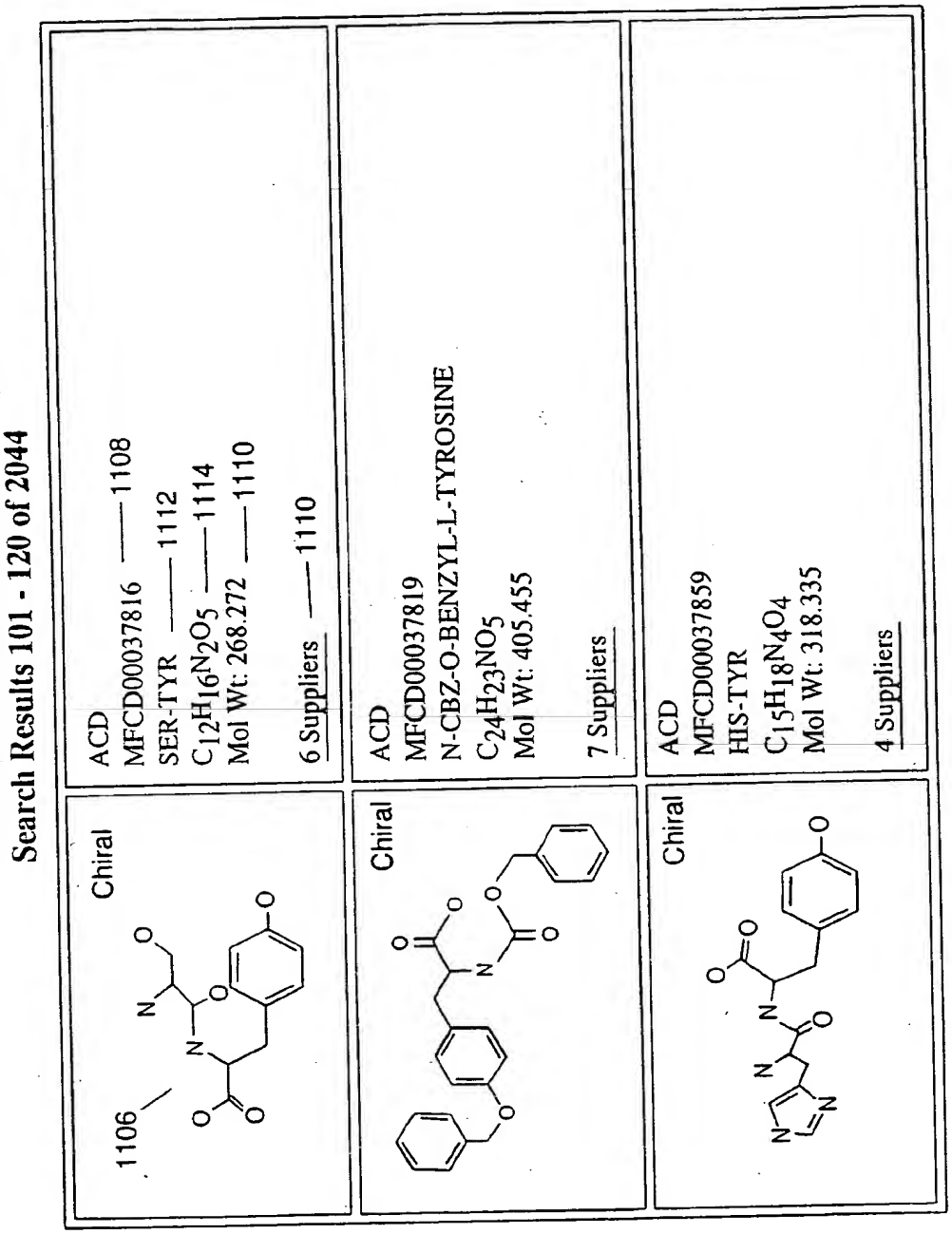

FIG. 11C

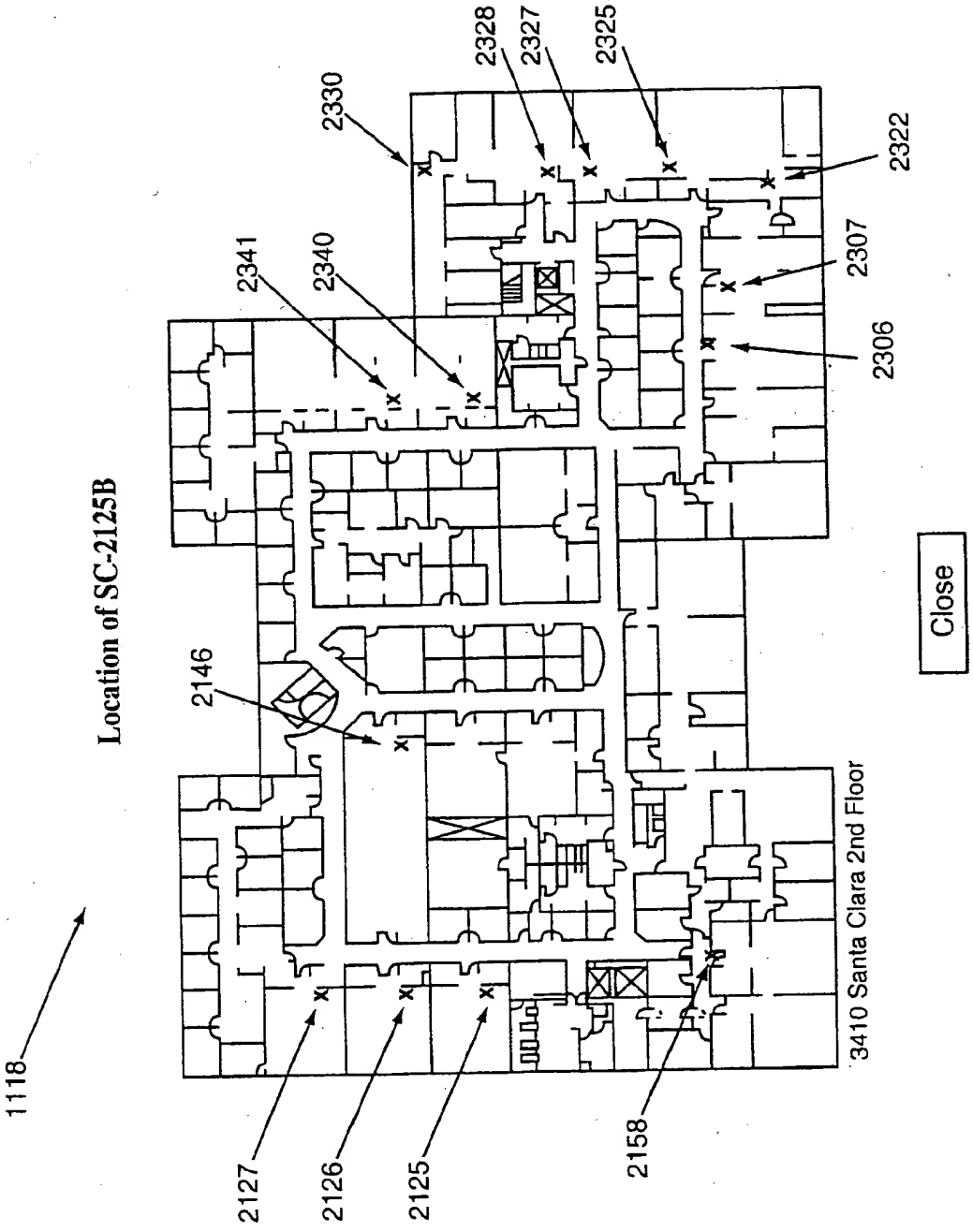

FIG. 11D

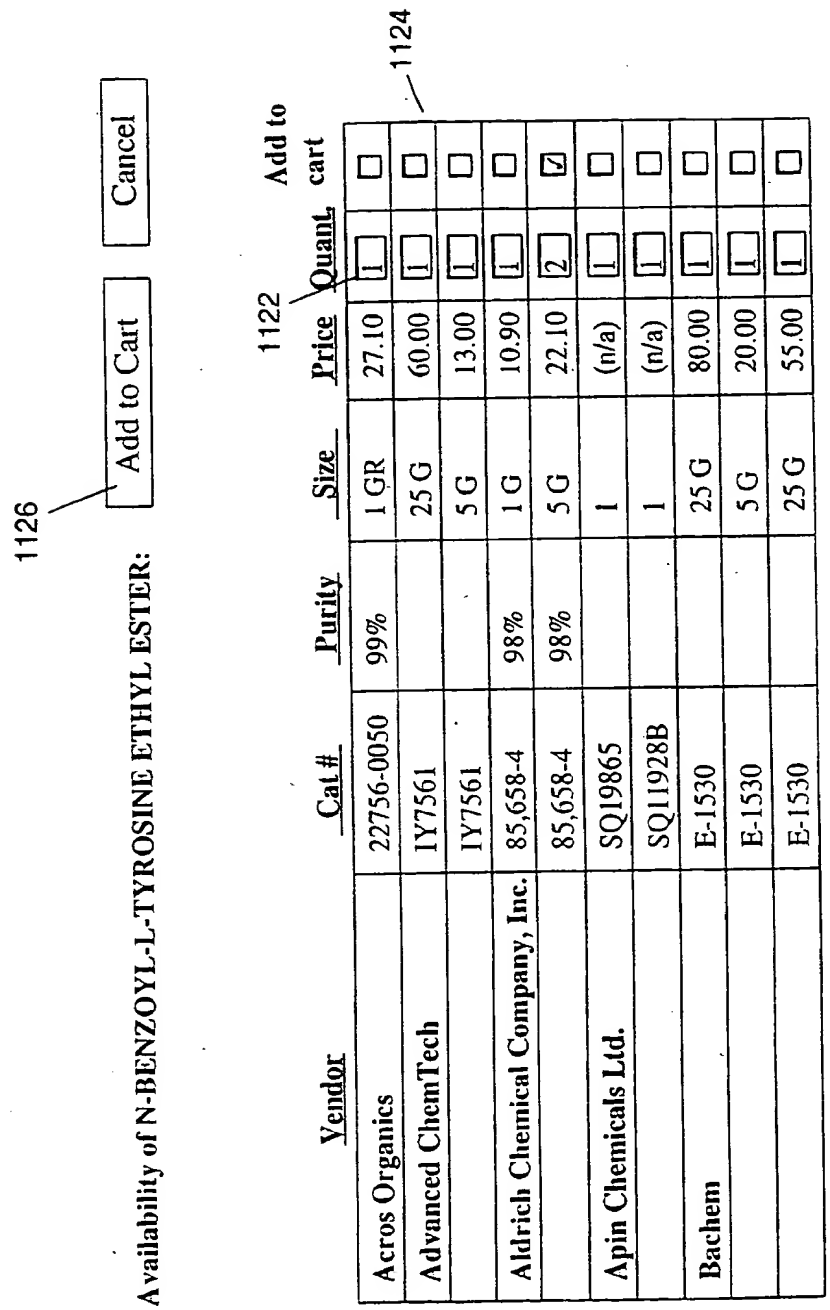

FIG. 11E

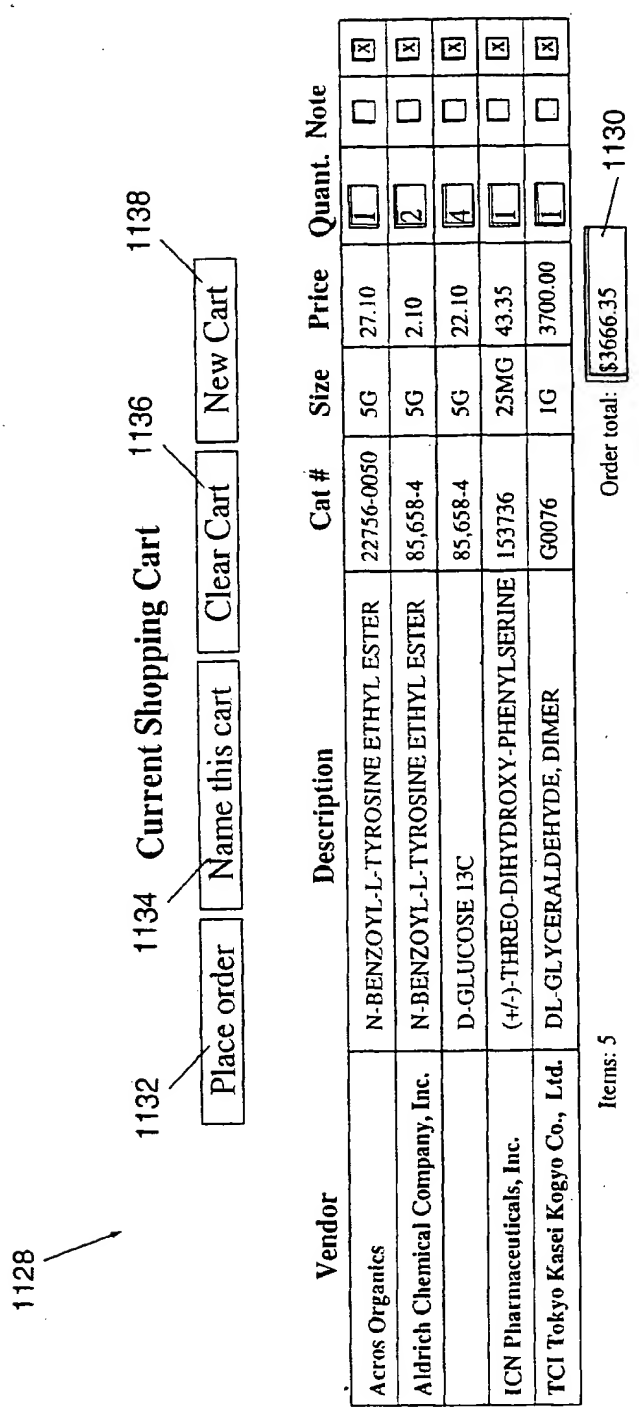

FIG. 11F

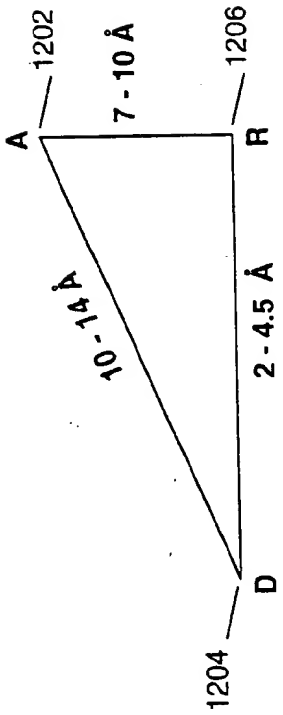

FIG. 12

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US99/15688

A. CLASSIFICATION OF SUBJECT MATTER
IPC(6) :G06F 17/30
US CL :707/1, 100
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 707/1, 100, 3

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

APS, CAS ONLINE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	US 5,577,239 A [MOORE ET AL.] 19 NOVEMBER 1996, SEE ABSTRACT	1-15
Y	US 5,321,804 A [KUSABA ET AL.] 14 JUNE 1994, SEE ABSTRACT	1-15
A, P,	US 5,787,279 A [RIGOUTSOS] 28 JULY 1998, SEE ABSTRACT	1
A	US 5,418,944 A [DIPACE ET AL.] 23 MAY 1995, SEE ENTIRE DOCUMENT	1
A, P	US 5,812,134 A [POOSER ET AL] 22 SEPTEMBER 1998, SEE ABSTRACT.	1

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

*	Special categories of cited documents:	"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"A"	document defining the general state of the art which is not considered to be of particular relevance	"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"E"	earlier document published on or after the international filing date	"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"&"	document member of the same patent family
"O"	document referring to an oral disclosure, use, exhibition or other means		
"P"	document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 27 AUGUST 1999	Date of mailing of the international search report 28 OCT 1999
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230	Authorized officer SANJIV SHAH FOR Telephone No. (703) 305-8355

Form PCT/ISA/210 (second sheet)(July 1992) *